JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1997, 119(16), 3732-3744, DOI:10.1021/ja963925g

A Model for the Structure of the Large-Pore Zeolite SSZ-31

Raul F. Lobo, Michael Tsapatsis, Clemens Freyhardt,

Ignatius Chan, Cong-Yan Chen, Stacey. I. Zones and Mark E. Davis

SUPLEMENTARY MATERIAL

Table A Atomic positional parameters of Polymorph C.
Table B Atomic positional parameters of Polymorph D.
Table C Atomic positional parameters of Polymorph E.
Table D Atomic positional parameters of Polymorph F.
Table E Atomic positional parameters of Polymorph G.
Table F Atomic positional parameters of Polymorph H.

Figure A. Structure-directing agents used for the synthesis of SSZ-31.
Figure B. Stacking sequence computed for $p=p_{\alpha\alpha'}=p_{\alpha'\alpha}=0.25$ for layers α and α'.
Figure C. Illustration of the stacking of layers α and β and the stacking vectors $\mathbf{R}_{ij}$. Note that the stacking vector $\mathbf{R}_{\beta\alpha'}$ also includes a translation of $1/2\underline{b}$. A translation of $1/2\underline{b}$ is equivalent to a change from Up to Down (and vice versa) in the configuration of the T atoms, i.e., O → ● and ● → O.
Figure D Effect of faulting on the X-ray powder diffraction pattern of Polymorph A.
Figure E Effect of faulting on the X-ray powder diffraction pattern of Polymorph C.
Figure F Effect of faulting on the X-ray powder diffraction pattern of Polymorph E.
Figure G Effect of faulting on the X-ray powder diffraction pattern of Polymorph G.
Figure H. XRD patterns of intergrowths of polymorphs A and C as a function of the stacking probability $p = p_{\alpha\beta} = 1 - p_{\beta\alpha}$.
Figure I. Schematic of the different polymorphs obtained as a function of *x* and *y*; the marked region indicate the approximate values for the crystallization of SSZ-31.
Figure J. Effect of the crystal size on the XRD pattern of intergrowths of layers α, α', β and β'. These calculations have been carried out using a value of

x=0.75 and y=0.1 and using u=0.1, v=-0.036 and w=0.01 as instrumental broadening parameters.

Figure K. Comparison of the trace of the synchrotron XRD pattern of SSZ-31 with the simulated XRD pattern of intergrowths of layers α, α', β and β' as that shows the best qualitative agreement. This pattern has been calculated with x=0.75, y=0.10, a crystal size of 1000 Å and using u=0.1, v=-0.036 and w=0.01 as instrumental broadening parameters.

Input data files for DIFFaX

A	Intergrowths of layers α, α', β and β'. Includes polymorphs A, B, C and D.
B	Intergrowths of layers γ, γ', δ and δ'. Includes polymorphs E, F, G and H.

Table A Atomic possitional parameters of Polymorph C, space group C2/m (No.12) a= 29.93 Å, b= 8.38 Å, c=12.35 Å, β=106 °.

Atom	Multiplicity and Wickof letter	x	y	z
Si1	8 j	0.0516	0.1866	0.9295
Si2	8 j	0.1910	0.1815	0.1253
Si3	8 j	0.1407	0.3153	0.8922
Si4	8 j	0.0467	0.3131	0.1592
Si5	8 j	0.1378	0.1843	0.3106
Si6	8 j	0.2903	0.6855	0.2368
Si7	8 j	0.2042	0.3146	0.5265
O1	4 i	0.0523	0.0000	0.9520
O2	4 i	0.1838	0.0000	0.0877
O3	4 i	0.1334	0.5000	0.8644
O4	4 i	0.0446	0.5000	0.1780
O5	4 i	0.1403	0.0000	0.3415
O6	4 i	0.2806	0.5000	0.2168
O7	4 i	0.2095	0.5000	0.5532
Oa	8 j	0.1651	0.2158	0.2192
Ob	8 j	0.2449	0.2171	0.1746
Oc	8 j	0.0916	0.2311	0.8727
Od	8 j	0.0850	0.2361	0.2614
Oe	8 j	0.0026	0.2362	0.8479
Of	8 j	0.1680	0.2366	0.8120
Og	4 f	0.2500	0.2500	0.5000
Oh	8 j	0.0599	0.2796	0.0453
Oi	8 j	0.1608	0.2855	0.4205
Oj	8 j	0.1700	0.2932	0.0196
Ok	8 j	0.3035	0.7225	0.3678

Table B Atomic positional parameters of Polymorph D, space group P bcm (No.57) a= 12.35 Å, b=28.78 Å, c= 8.38 Å.

Atom	Multiplicity and Wickof letter	x	y	z
Si 1	8e	0.2155	0.0415	0.0649
Si 2	8e	0.1567	0.9434	0.9370
Si 3	8e	0.0496	0.1065	0.9310
Si 4	8e	0.4551	0.0495	0.9405
Si 5	8e	0.3663	0.8850	0.9365
Si 6	8e	0.9645	0.1985	0.0629
Si 7	8e	0.7330	0.2015	0.9360
O 1	4d	0.2344	0.0282	0.2500
O 2	4d	0.1319	0.9352	0.7500
O 3	4d	0.0900	0.0986	0.7500
O 4	4d	0.4715	0.0541	0.7500
O 5	4d	0.3580	0.8714	0.7500
O 6	4d	0.9939	0.1946	0.2500
O 7	4d	0.7647	0.2064	0.7500
Oa	4c	0.9917	0.2500	0.0000
Ob	4c	0.6852	0.2500	0.0000
Oc	4b	0.5000	0.0000	0.0000
Od	8e	0.0633	0.9199	0.0429
Oe	8e	0.5197	0.0905	0.0294
Of	8e	0.8384	0.1881	0.0380
Og	8e	0.3561	0.8387	0.0437
Oh	8e	0.1375	0.0860	0.0536
O i	8e	0.0340	0.1612	0.9633
O j	8e	0.1609	0.9983	0.9734
Ok	8e	0.2706	0.9203	0.9818
Ol	8e	0.3291	0.0535	0.9825

Table C Atomic positional parameters of Polymorph E (C/2m (No. 12)).

Atom	x	y	z
Si 1	0.6347	0.3121	0.9124
Si 2	0.4873	0.1838	0.0988
Si 3	0.6759	0.1856	0.4117
Si 4	0.3988	0.3147	0.7722
Si 5	0.7043	0.3139	0.6004
Si 6	0.6806	0.1847	0.1135
Si 7	0.2986	0.1837	0.2179
O 1	0.5380	0.2612	0.1772
O 2	0.2553	0.2079	0.8270
O 3	0.6403	0.2837	0.1602
O 4	0.7670	0.2548	0.6080
O 5	0.6435	0.5000	0.9061
O 6	0.4812	0.0000	0.1224
O 7	0.4300	0.2754	0.0959
O 8	0.5000	0.1986	0.0000
O 9	0.6022	0.5000	0.2528
O 10	0.3269	0.2472	0.9902
O 11	0.6809	0.0000	0.4367
O 12	0.6244	0.2137	0.3212
O 13	0.2949	0.5000	0.3766
O 14	0.2819	0.0000	0.2007
O 15	0.3202	0.2175	0.3272
O 16	0.3476	0.2255	0.1706
O 17	0.6645	0.0000	0.1109
O 18	0.3347	0.2833	0.5029

Table D Atomic positional parameters of Polymorph F (Cmca (No. 64)).

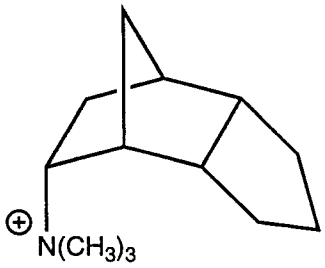
Atom	x	y	z
Si 1	0.6829	0.2735	0.3920
Si 2	0.8145	0.3564	0.4610
Si 3	0.8230	0.4757	0.0515
Si 4	0.6906	0.2275	0.1996
Si 5	0.8095	0.6063	0.1997
Si 6	0.6818	0.1730	0.0584
Si 7	0.6845	0.5703	0.1077
O 1	0.0000	0.6036	0.1975
O 2	0.7102	0.6153	0.4178
O 3	0.7191	0.3312	0.5040
O 4	0.5000	0.2919	0.3942
O 5	0.0000	0.1909	0.4343
O 6	0.7032	0.2170	0.4184
O 7	0.7500	0.5877	0.2500
O 8	0.7918	0.3183	0.4165
O 9	0.5000	0.2301	0.1975
O 10	0.7483	0.6669	0.3101
O 11	0.0000	0.3603	0.4736
O 12	0.0000	0.5864	0.3957
O 13	0.7643	0.5668	0.3388
O 14	0.7500	0.2460	0.2500
O 15	0.7878	0.5129	0.4165
O 16	0.6725	0.5000	0.5000
O 17	0.7359	0.2668	0.3389
O 18	0.5000	0.4744	0.4277
O 19	0.7473	0.4155	0.4499

Table E Atomic positional parameters of Polymorph G (C/2m (No. 12)).

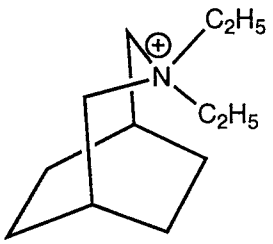
Atom	x	y	z
Si 1	0.1633	0.3134	0.3970
Si 2	0.2327	0.3157	0.7759
Si 3	0.8091	0.1855	0.0916
Si 4	0.7830	0.1869	0.4067
Si 5	0.9219	0.3146	0.0806
Si 6	0.8785	0.3185	0.8822
Si 7	0.0554	0.1847	0.2186
O 1	0.2197	0.5000	0.7808
O 2	0.5898	0.2068	0.1600
O 3	0.8171	0.0000	0.0810
O 4	0.5924	0.2829	0.0102
O 5	0.7500	0.7500	0.0000
O 6	0.9223	0.5000	0.0612
O 7	0.2874	0.2204	0.6201
O 8	0.7958	0.2639	0.3302
O 9	0.0122	0.2634	0.8362
O 10	0.3057	0.2842	0.8305
O 11	0.9514	0.0000	0.7671
O 12	0.8901	0.5000	0.8678
O 13	0.9054	0.2689	0.6834
O 14	0.1715	0.2638	0.4951
O 15	0.7945	0.0000	0.4110
O 16	0.2008	0.2145	0.8219
O 17	0.1738	0.5000	0.3956
O 18	0.8697	0.2775	0.1071

Table F Atomic positional parameters of Polymorph G (Cmca, No. 64).

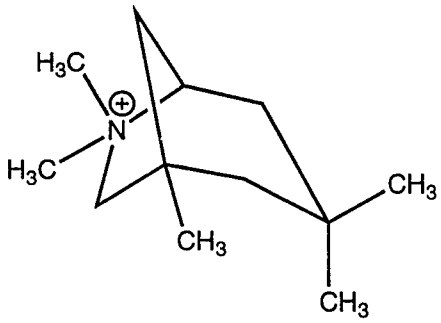
Atom	x	y	z
Si 1	0.6833	0.5231	0.3939
Si 2	0.8145	0.6119	0.4546
Si 3	0.8118	0.7306	0.0499
Si 4	0.6805	0.4859	0.2003
Si 5	0.8195	0.8573	0.2003
Si 6	0.6853	0.4218	0.0506
Si 7	0.6828	0.8247	0.1058
O 1	0.0000	0.8368	0.1958
O 2	0.7044	0.8663	0.4213
O 3	0.7383	0.5849	0.5000
O 4	0.5000	0.5385	0.4021
O 5	0.0000	0.4363	0.4542
O 6	0.7250	0.4693	0.4222
O 7	0.7500	0.8406	0.2500
O 8	0.7943	0.5716	0.4115
O 9	0.5000	0.5064	0.1958
O 10	0.6858	0.9216	0.3051
O 11	0.0000	0.6233	0.4633
O 12	0.0000	0.8381	0.4054
O 13	0.7867	0.8301	0.3396
O 14	0.7500	0.5027	0.2500
O 15	0.7776	0.7643	0.4105
O 16	0.7500	0.7500	0.5000
O 17	0.7136	0.5131	0.3397
O 18	0.5000	0.7406	0.4464
O 19	0.7253	0.6676	0.4436



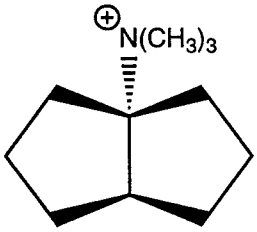
1



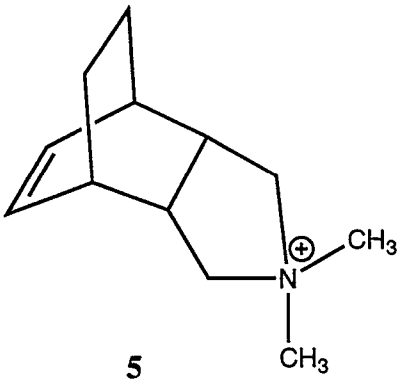
2



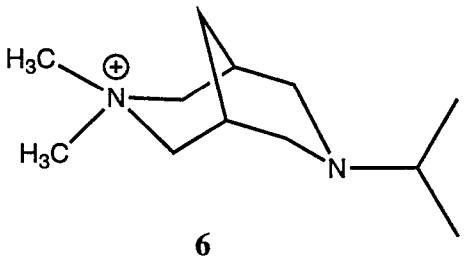
3



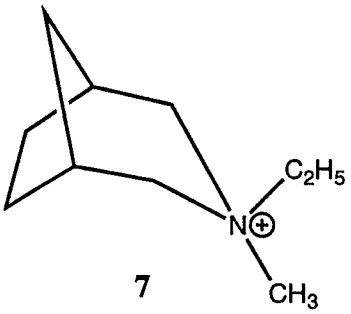
4



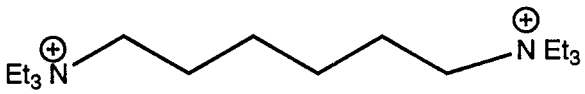
5



6



7



8

Fig A

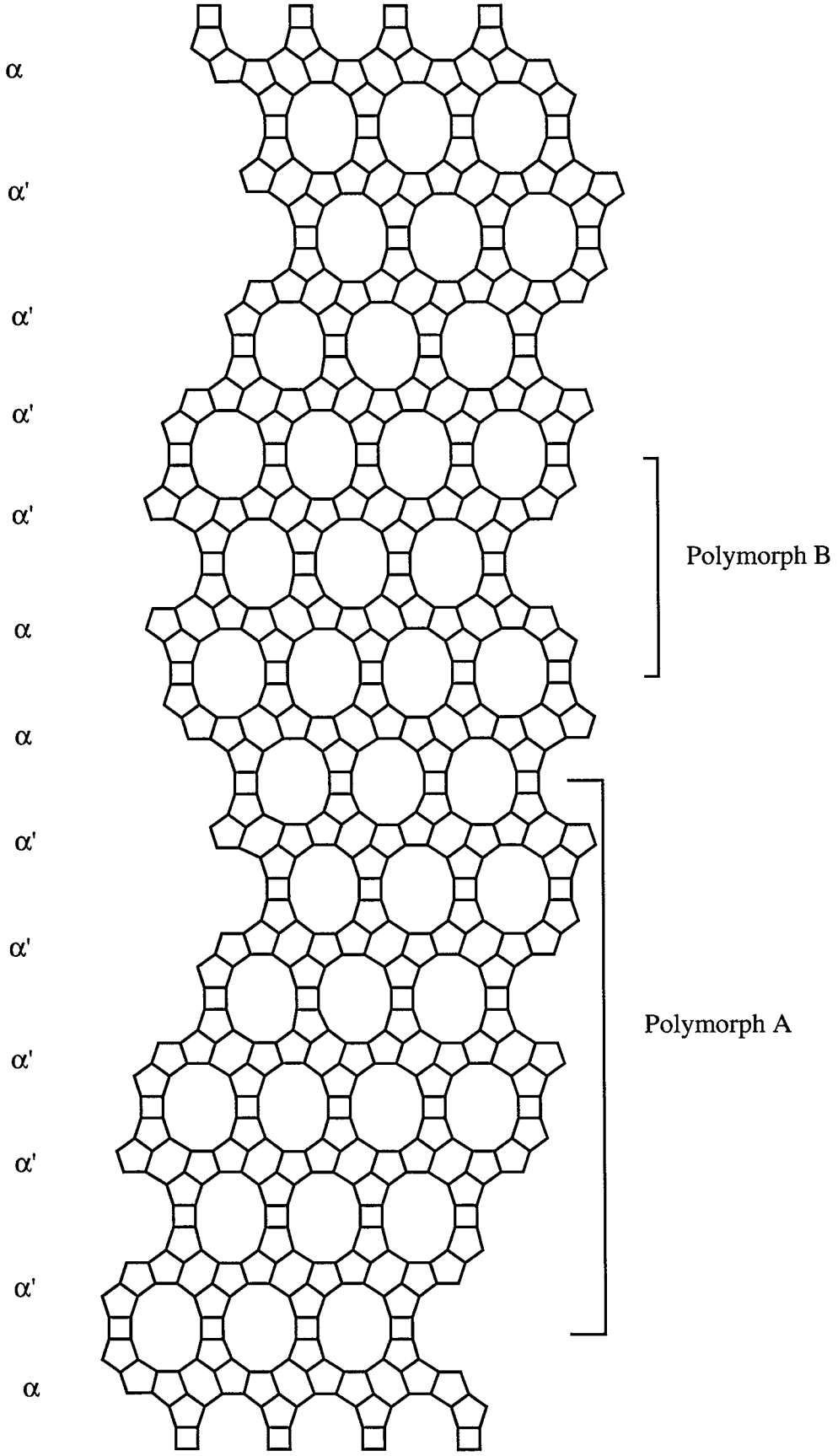


Fig B

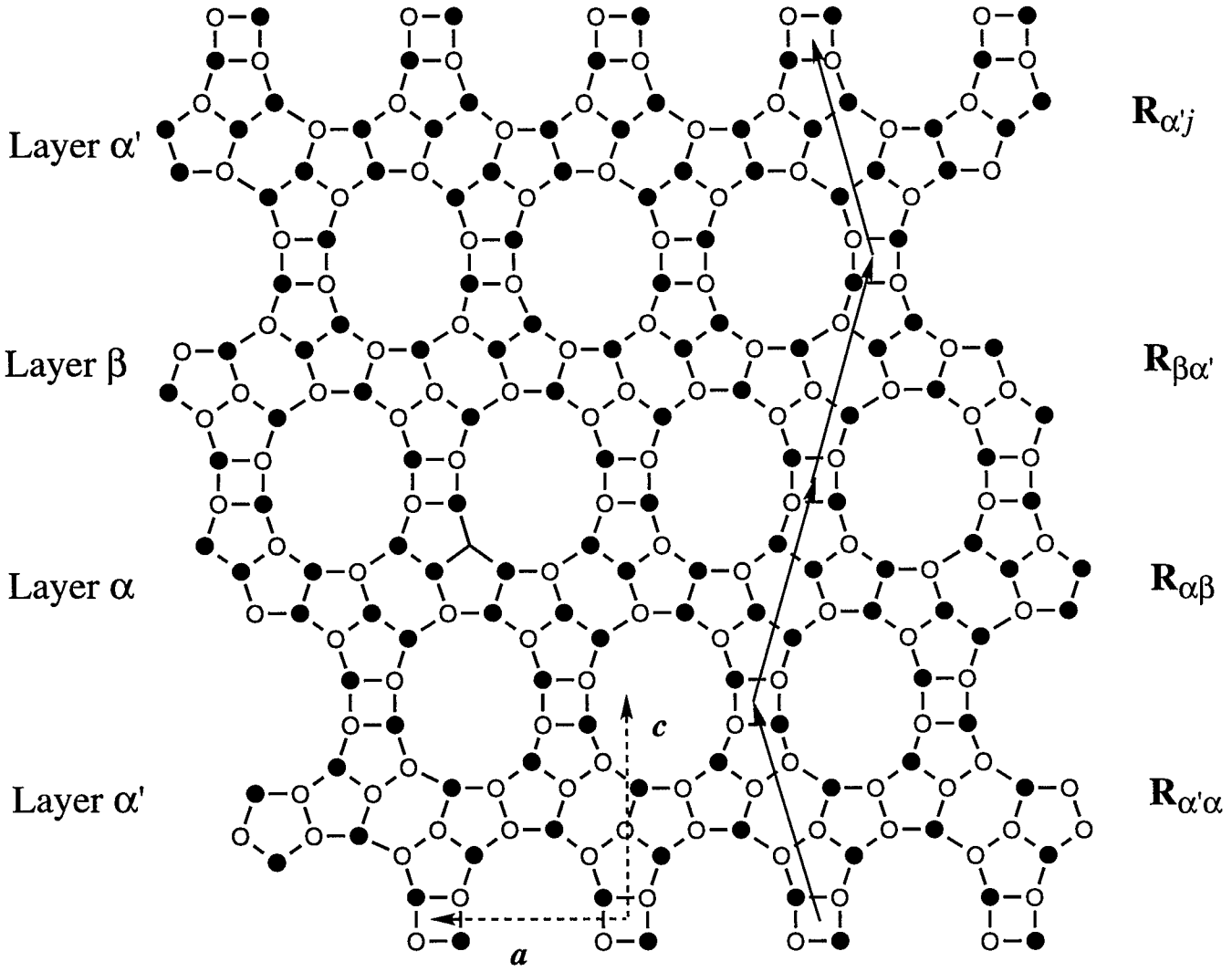

Layer α'
Layer β
Layer α
Layer α'
$\mathbf{R}_{\alpha' j}$
$\mathbf{R}_{\beta\alpha'}$
$\mathbf{R}_{\alpha\beta}$
$\mathbf{R}_{\alpha'\alpha}$
c
a

Fig C

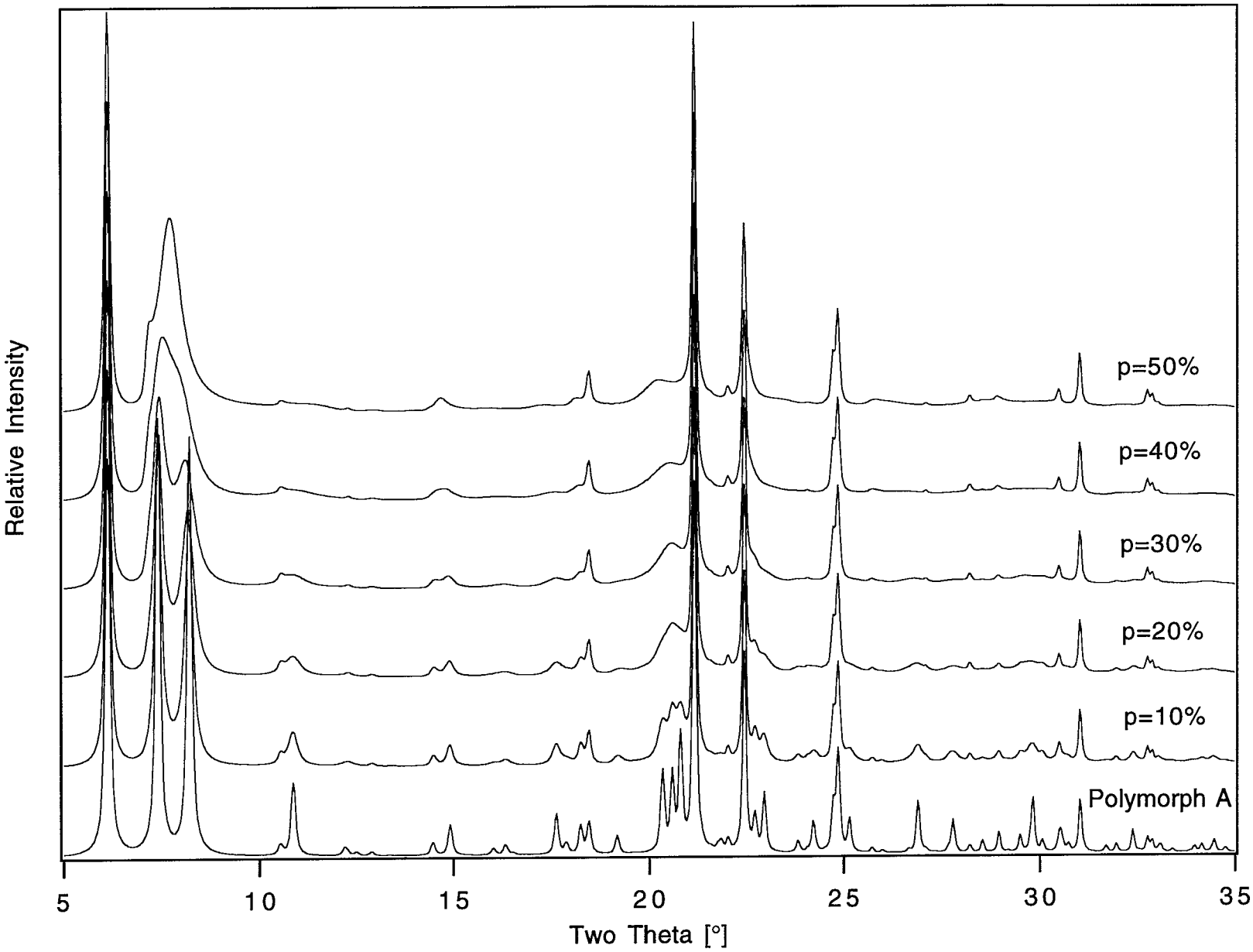

Relative Intensity
p=50%
p=40%
p=30%
p=20%
p=10%
Polymorph A
5
10
15
20
25
30
35
Two Theta [°]

Figure D

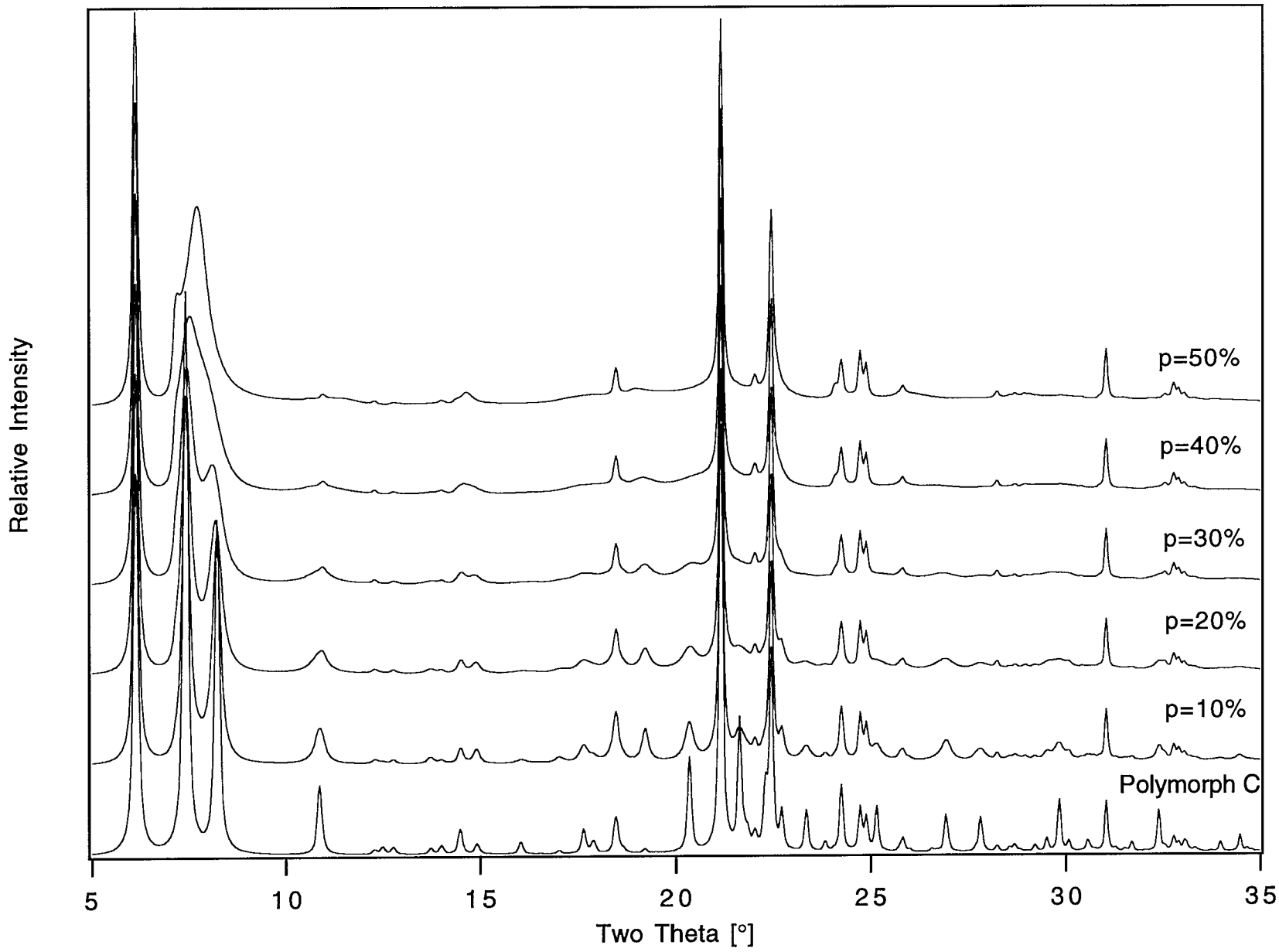

Relative Intensity
p=50%
p=40%
p=30%
p=20%
p=10%
Polymorph C
5
10
15
20
25
30
35
Two Theta [°]

Figure E

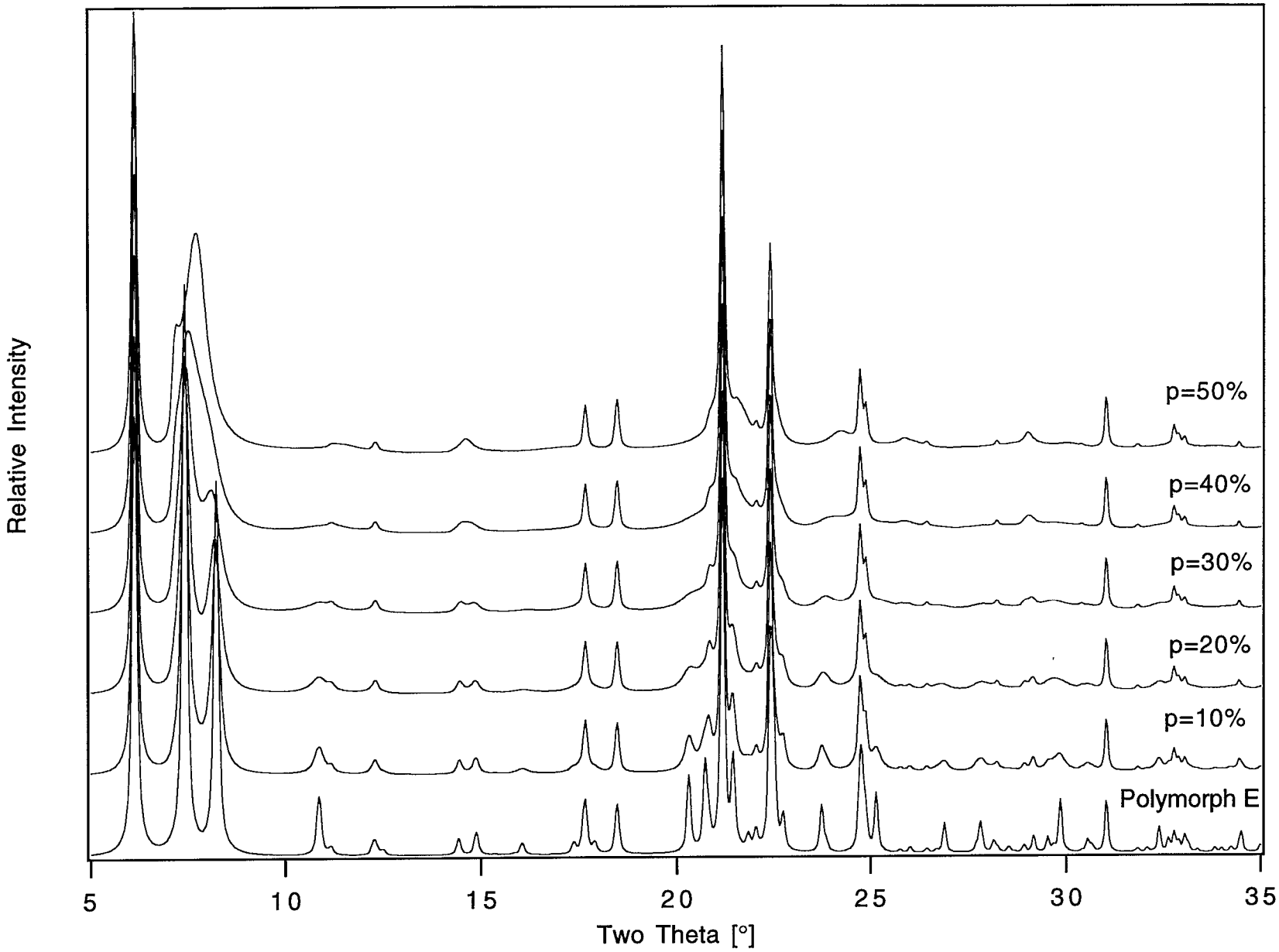

Relative Intensity
p=50%
p=40%
p=30%
p=20%
p=10%
Polymorph E
5
10
15
20
25
30
35
Two Theta [°]

Figure F

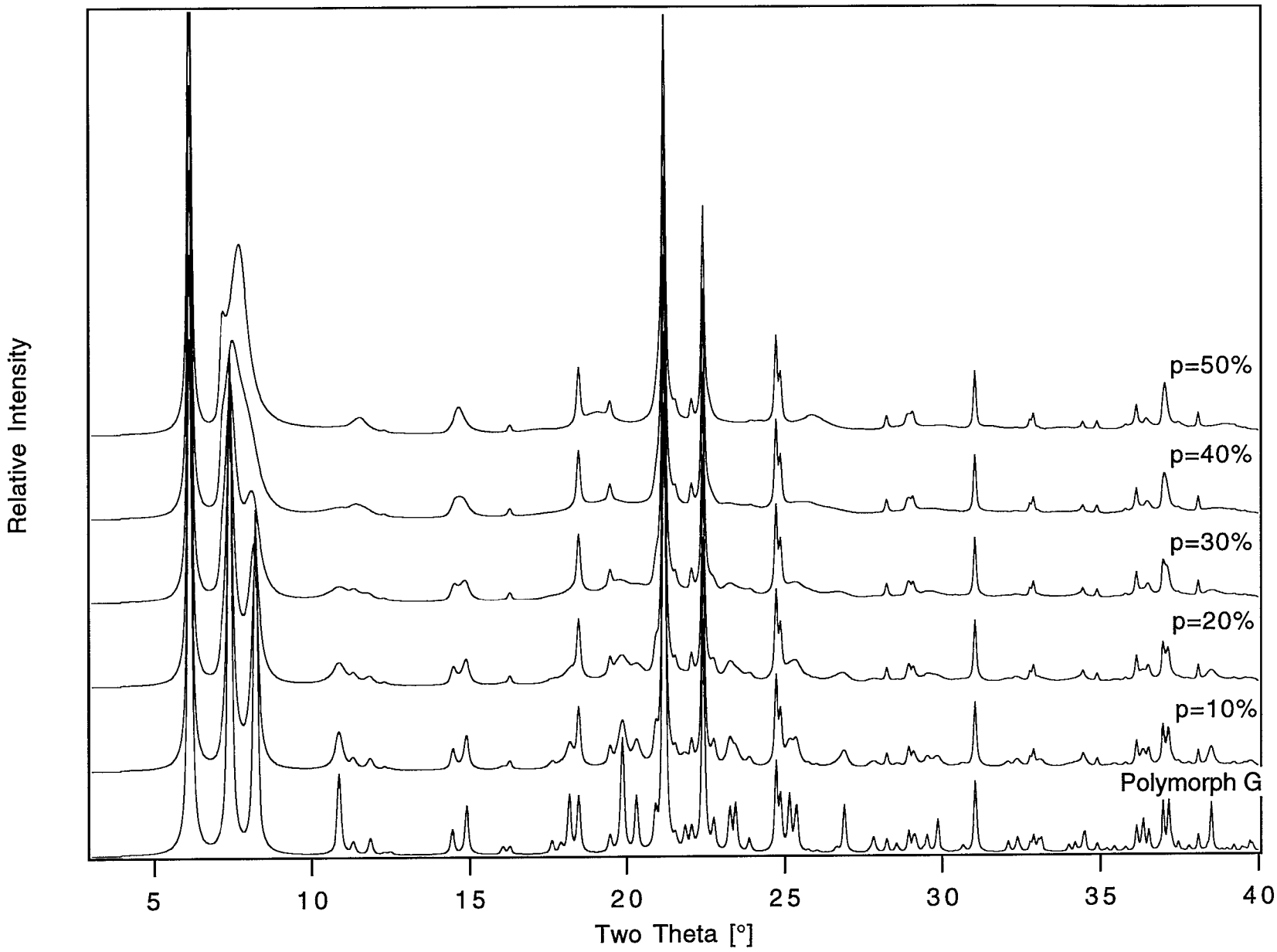

Relative Intensity
p=50%
p=40%
p=30%
p=20%
p=10%
Polymorph G
5
10
15
20
25
30
35
40
Two Theta [°]

Figure 6

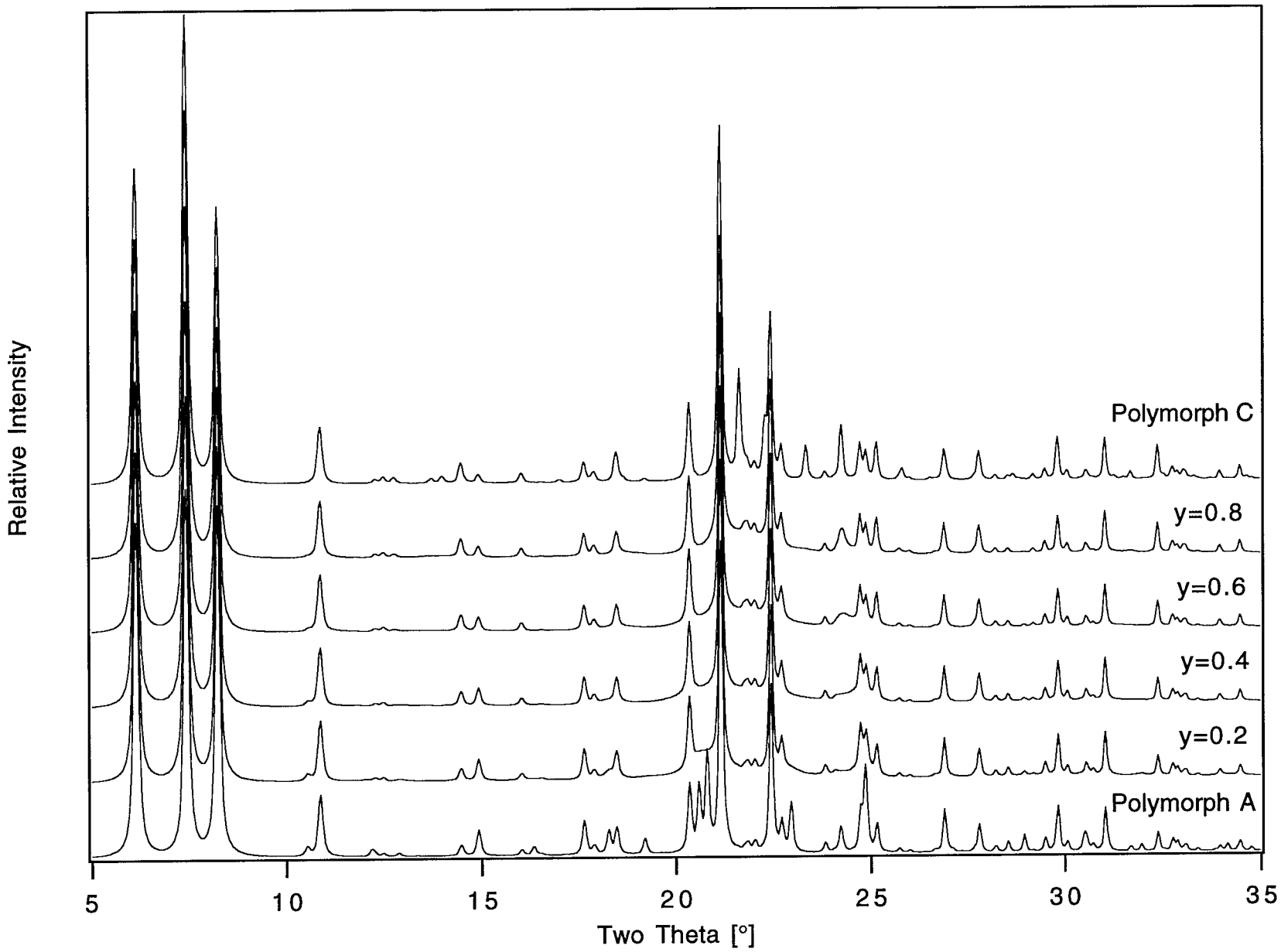

Relative Intensity
Polymorph C
y=0.8
y=0.6
y=0.4
y=0.2
Polymorph A
5
10
15
20
25
30
35
Two Theta [°]

Fig H

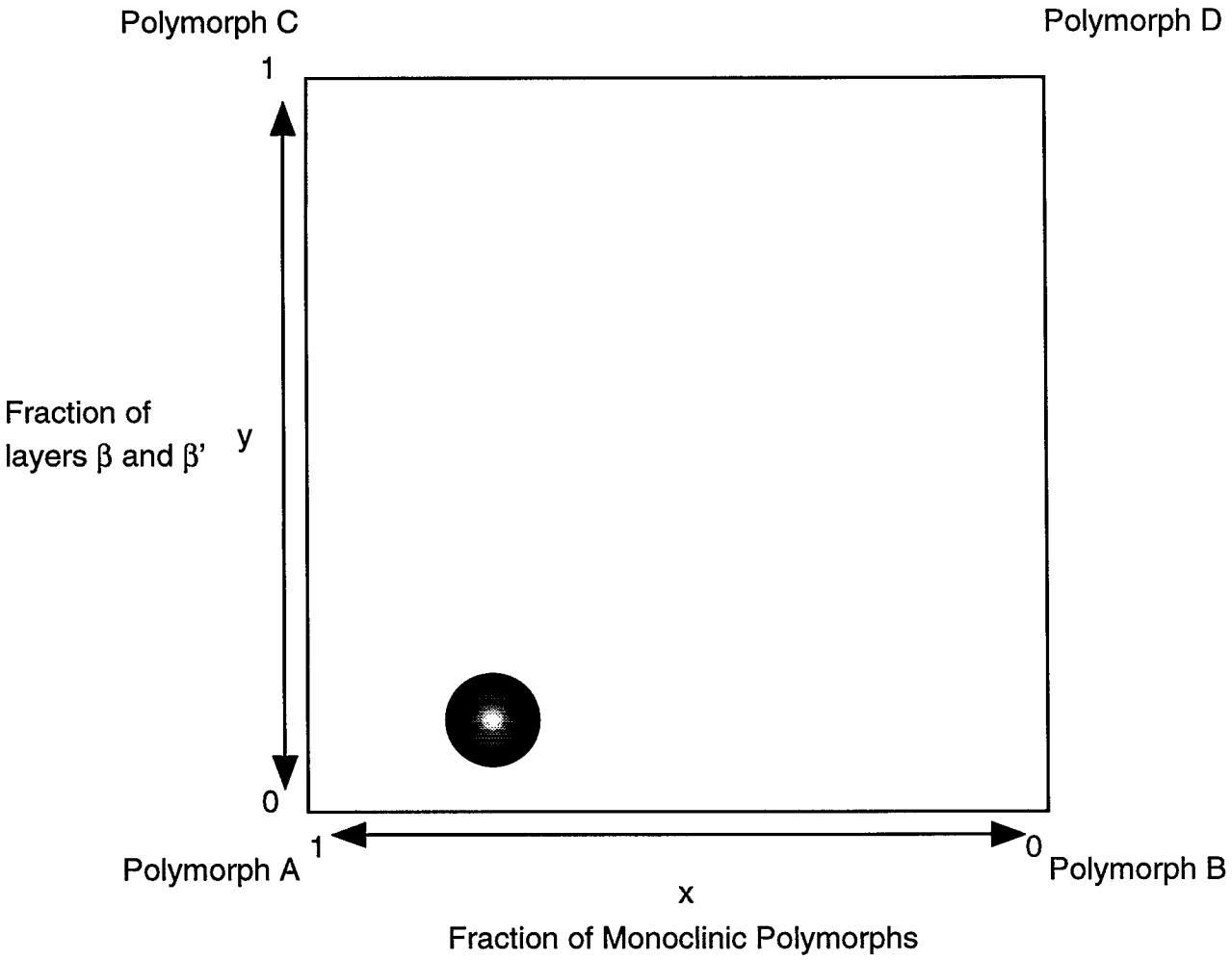

Polymorph C
Polymorph D
1
Fraction of
layers β and β'
y
0
1
0
Polymorph A
Polymorph B
x
Fraction of Monoclinic Polymorphs

Fig I

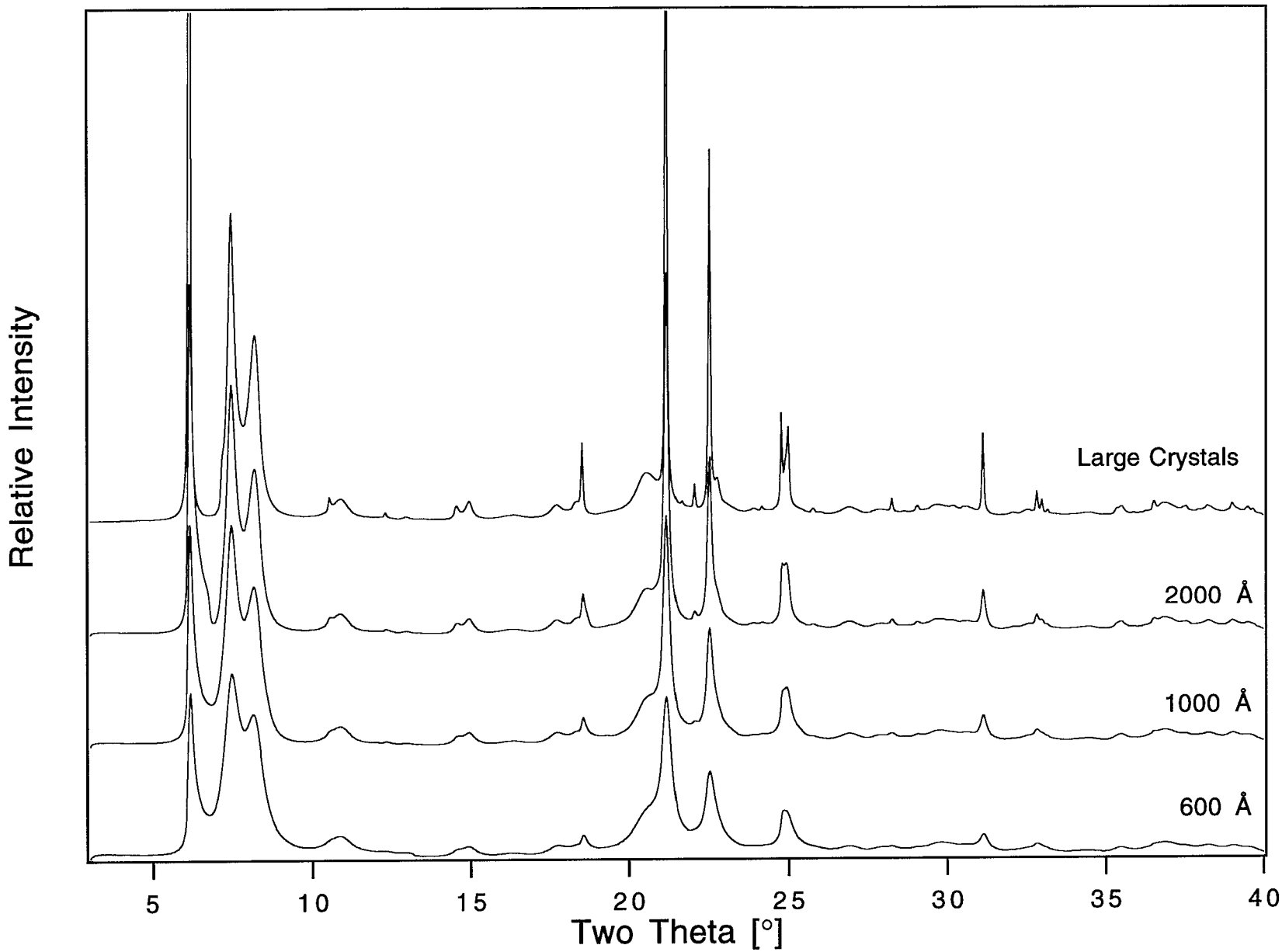

Relative Intensity
Large Crystals
2000 Å
1000 Å
600 Å
5
10
15
20
25
30
35
40
Two Theta [°]

Fig J

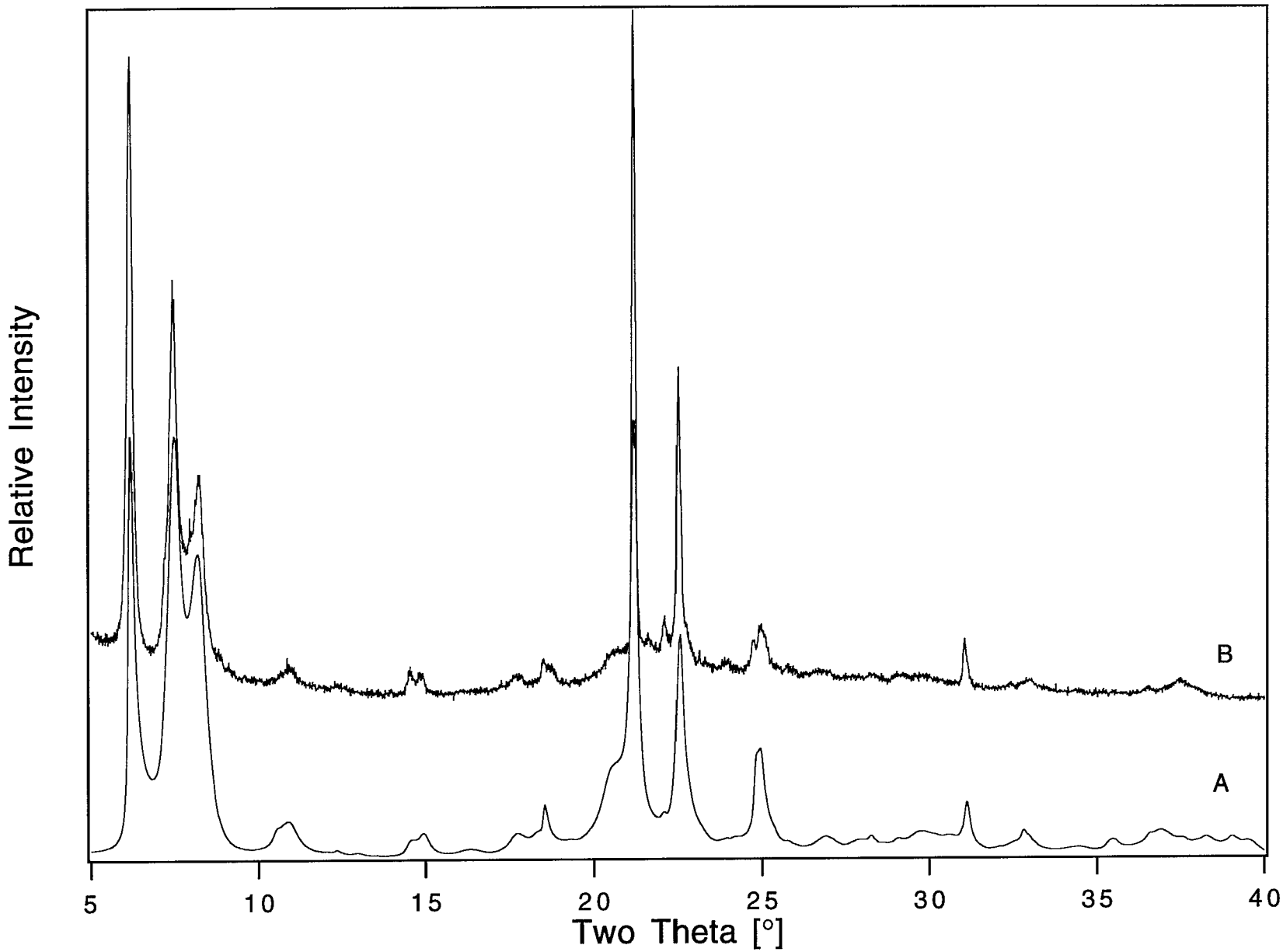


Fig K

```
{THIS IS AN INPUT FILE FOR THE PROGRAM DIFFaX}
{This input file can be used to simulate intergrowths of layers alpha, alpha}
{beta and beta'. This file has been provided as supplementary material for}
{the paper "A Model for the Structure of the Large-Pore Zeolite SSZ-31"}
{J. Am. Chem. Soc., 1997}
{See the text of the paper for more details}

{Layer 1= layer alpha}
{Layer 2= layer alpha'}
{Layer 3= layer beta}
{Layer 4= layer beta'}

{To simulate intergrowths of polymorphs A and B, }
{then the stacking transitions are defined as:}
{1-1  is a polymorph A stacking transition}
{1-2  is a polymorph B stacking transition}
{1-3 cannot occur}
{1-4 cannot occur}
{2-1  is a polymorph B stacking transition}
{2-2  is a polymorph A stacking transition}
{2-3 cannot occur}
{2-4 cannot occur}
{3-i cannot occur, i=1,2,3,4}
{4-i cannot occur, i=1,2,3,4}
{Remember that the program requires that the sum of the stacking}
{transitions for each layer equal to one}

{To simulate intergrowths of polymorphs C and D, }
{then the stacking transitions are defined as:}
{1-i cannot occur, i=1,2,3,4}
{2-i cannot occur, i=1,2,3,4}
{3-1 cannot occur}
{3-2 cannot occur}
{3-3  is a polymorph C stacking transition}
{3-4  is a polymorph D stacking transition}
{4-1 cannot occur}
{4-2 cannot occur}
{4-3  is a polymorph D stacking transition}
{4-4  is a polymorph C stacking transition}

{To simulate intergrowths that include layers alpha, alpha', beta and beta'}
{it is necessary to define the stacking transition probabilities according}
{to the constrains discussed in the text of the paper}
{To run a simulation with the parameters x=0.75 and y=0.1 use the following}
{lines as the stacking transitions data}

{layer 1}
{{to layer 1} 0.675   -0.3333  0.0    1.0}
{{to layer 2} 0.225   -0.3333  0.0    1.0}
{{to layer 3} 0.075   -0.3333  0.0    1.0}
{{to layer 4} 0.025   -0.3333  0.0    1.0}
{layer 2}
{{to layer 1} 0.225    0.3333  0.0    1.0}
{{to layer 2} 0.675    0.3333  0.0    1.0}
{{to layer 3} 0.025    0.3333  0.0    1.0}
{{to layer 4} 0.075    0.3333  0.0    1.0}
{layer 3}
{{to layer 1} 0.675   -0.3333  0.5    1.0}
{{to layer 2} 0.225   -0.3333  0.5    1.0}
{{to layer 3} 0.075   -0.3333  0.5    1.0}
```

```
{{to layer 4} 0.025   -0.3333  0.5    1.0}
{layer 4}
{{to layer 1} 0.225    0.3333  0.5    1.0}
{{to layer 2} 0.675    0.3333  0.5    1.0}
{{to layer 3} 0.025    0.3333  0.5    1.0}
{{to layer 4} 0.075    0.3333  0.5    1.0}


INSTRUMENTAL
X-RAY
1.5418
NONE

STRUCTURAL
12.35  8.4  14.4  90.0
UNKNOWN 1.0                  {}
4

LAYER 1  {This is layer alpha}
{Structural data obtained from the DLS-76 optimized atomic positions of}
{polymorph B.  Consecutive stackings of this layer forms polymorph A}
NONE
Si4+    1   0.5642  0.3110  0.9025  1.00    1.00
Si4+    2   0.8046  0.1886  0.9011  1.00    1.00
Si4+    3   0.2240  0.1845  0.2781  1.00    1.00
Si4+    4   0.2809  0.3143  0.5929  1.00    1.00
Si4+    5   0.6550  0.3185  0.6181  1.00    1.00
Si4+    6   0.8792  0.3144  0.7155  1.00    1.00
Si4+    7   0.5642  0.6890  0.9025  1.00    1.00
Si4+    8   0.0474  0.1822  0.5756  1.00    1.00
Si4+    9   0.8046  0.8114  0.9011  1.00    1.00
Si4+    10  0.1177  0.3110  0.0975  1.00    1.00
Si4+    11  0.8773  0.1886  0.0989  1.00    1.00
Si4+    12  0.4579  0.1845  0.7219  1.00    1.00
Si4+    13  0.4010  0.3143  0.4071  1.00    1.00
Si4+    14  0.0269  0.3185  0.3819  1.00    1.00
Si4+    15  0.8027  0.3144  0.2845  1.00    1.00
Si4+    16  0.6345  0.1822  0.4244  1.00    1.00
Si4+    17  0.2240  0.8155  0.2781  1.00    1.00
Si4+    18  0.2809  0.6858  0.5929  1.00    1.00
Si4+    19  0.1177  0.6890  0.0975  1.00    1.00
Si4+    20  0.8773  0.8114  0.0989  1.00    1.00
Si4+    21  0.4579  0.8155  0.7219  1.00    1.00
Si4+    22  0.4010  0.6858  0.4071  1.00    1.00
Si4+    23  0.6550  0.6815  0.6181  1.00    1.00
Si4+    24  0.0269  0.6815  0.3819  1.00    1.00
Si4+    25  0.8027  0.6856  0.2845  1.00    1.00
Si4+    26  0.6345  0.8178  0.4244  1.00    1.00
Si4+    27  0.8792  0.6856  0.7155  1.00    1.00
Si4+    28  0.0474  0.8178  0.5756  1.00    1.00
O 1-    1   0.0121  0.7088  0.4905  1.00    1.00
O 1-    2   0.6819  0.2397  0.8849  1.00    1.00
O 1-    3   0.1971  0.2540  0.1779  1.00    1.00
O 1-    4   0.3562  0.2758  0.6798  1.00    1.00
O 1-    5   0.5597  0.2082  0.6556  1.00    1.00
O 1-    6   0.8785  0.2647  0.8221  1.00    1.00
O 1-    7   0.9714  0.7818  0.6624  1.00    1.00
O 1-    8   0.7646  0.2748  0.6704  1.00    1.00
O 1-    9   0.1700  0.2192  0.6023  1.00    1.00
```

O 1-	10	0.0121	0.2912	0.4905	1.00	1.00
O 1-	11	0.9714	0.2182	0.6624	1.00	1.00
O 1-	12	0.1620	0.2500	0.0000	1.00	1.00
O 1-	13	0.0000	0.2397	0.1151	1.00	1.00
O 1-	14	0.8379	0.2500	0.0000	1.00	1.00
O 1-	15	0.4848	0.2540	0.8221	1.00	1.00
O 1-	16	0.3257	0.2758	0.3202	1.00	1.00
O 1-	17	0.3410	0.2619	0.5000	1.00	1.00
O 1-	18	0.1222	0.2082	0.3444	1.00	1.00
O 1-	19	0.8034	0.2647	0.1779	1.00	1.00
O 1-	20	0.9173	0.2748	0.3296	1.00	1.00
O 1-	21	0.5119	0.2192	0.3977	1.00	1.00
O 1-	22	0.6698	0.2912	0.5095	1.00	1.00
O 1-	23	0.7105	0.2182	0.3376	1.00	1.00
O 1-	24	0.1115	0.5000	0.0969	1.00	1.00
O 1-	25	0.0000	0.7604	0.1151	1.00	1.00
O 1-	26	0.8678	0.0000	0.1029	1.00	1.00
O 1-	27	0.4308	0.0000	0.7303	1.00	1.00
O 1-	28	0.4848	0.7460	0.8221	1.00	1.00
O 1-	29	0.3257	0.7242	0.3202	1.00	1.00
O 1-	30	0.4253	0.5000	0.4105	1.00	1.00
O 1-	31	0.0562	0.5000	0.3629	1.00	1.00
O 1-	32	0.1222	0.7918	0.3444	1.00	1.00
O 1-	33	0.8034	0.7353	0.1779	1.00	1.00
O 1-	34	0.9173	0.7252	0.3296	1.00	1.00
O 1-	35	0.7795	0.5000	0.2931	1.00	1.00
O 1-	36	0.5119	0.7809	0.3977	1.00	1.00
O 1-	37	0.6458	0.0000	0.4527	1.00	1.00
O 1-	38	0.6698	0.7088	0.5095	1.00	1.00
O 1-	39	0.7105	0.7818	0.3376	1.00	1.00
O 1-	40	0.1620	0.7500	0.0000	1.00	1.00
O 1-	41	0.8379	0.7500	0.0000	1.00	1.00
O 1-	42	0.5704	0.5000	0.9031	1.00	1.00
O 1-	43	0.6819	0.7604	0.8849	1.00	1.00
O 1-	44	0.8141	0.0000	0.8971	1.00	1.00
O 1-	45	0.2511	0.0000	0.2697	1.00	1.00
O 1-	46	0.1971	0.7460	0.1779	1.00	1.00
O 1-	47	0.3562	0.7242	0.6798	1.00	1.00
O 1-	48	0.3410	0.7381	0.5000	1.00	1.00
O 1-	49	0.2566	0.5000	0.5895	1.00	1.00
O 1-	50	0.6258	0.5000	0.6371	1.00	1.00
O 1-	51	0.5597	0.7918	0.6556	1.00	1.00
O 1-	52	0.8785	0.7353	0.8221	1.00	1.00
O 1-	53	0.7646	0.7252	0.6704	1.00	1.00
O 1-	54	0.9024	0.5000	0.7069	1.00	1.00
O 1-	55	0.1700	0.7809	0.6023	1.00	1.00
O 1-	56	0.0361	0.0000	0.5473	1.00	1.00

LAYER 2 {This is layer alpha'}
{Structural data obtained from the DLS-76 optimized atomic positions of}
{polymorph B}
NONE

Si4+	1	0.4358	0.8110	0.9025	1.00	1.00
Si4+	2	0.1954	0.6886	0.9011	1.00	1.00
Si4+	3	0.4358	0.1890	0.9025	1.00	1.00
Si4+	4	0.1954	0.3114	0.9011	1.00	1.00
Si4+	5	0.7760	0.3155	0.2781	1.00	1.00
Si4+	6	0.7191	0.1858	0.5929	1.00	1.00
Si4+	7	0.3450	0.1815	0.6181	1.00	1.00

Si4+	8	0.1208	0.1856	0.7155	1.00	1.00
Si4+	9	0.7760	0.6845	0.2781	1.00	1.00
Si4+	10	0.9526	0.3178	0.5756	1.00	1.00
Si4+	11	0.7191	0.8143	0.5929	1.00	1.00
Si4+	12	0.8823	0.1890	0.0975	1.00	1.00
Si4+	13	0.1227	0.3114	0.0989	1.00	1.00
Si4+	14	0.5421	0.3155	0.7219	1.00	1.00
Si4+	15	0.5990	0.1858	0.4071	1.00	1.00
Si4+	16	0.9731	0.1815	0.3819	1.00	1.00
Si4+	17	0.1973	0.1856	0.2845	1.00	1.00
Si4+	18	0.3655	0.3178	0.4244	1.00	1.00
Si4+	19	0.3450	0.8185	0.6181	1.00	1.00
Si4+	20	0.1208	0.8144	0.7155	1.00	1.00
Si4+	21	0.8823	0.8110	0.0975	1.00	1.00
Si4+	22	0.1227	0.6886	0.0989	1.00	1.00
Si4+	23	0.5421	0.6845	0.7219	1.00	1.00
Si4+	24	0.5990	0.8143	0.4071	1.00	1.00
Si4+	25	0.9526	0.6822	0.5756	1.00	1.00
Si4+	26	0.9731	0.8185	0.3819	1.00	1.00
Si4+	27	0.1973	0.8144	0.2845	1.00	1.00
Si4+	28	0.3655	0.6822	0.4244	1.00	1.00
O 1-	1	0.3181	0.2604	0.8849	1.00	1.00
O 1-	2	0.8029	0.2460	0.1779	1.00	1.00
O 1-	3	0.6438	0.2242	0.6798	1.00	1.00
O 1-	4	0.4403	0.2918	0.6556	1.00	1.00
O 1-	5	0.1215	0.2353	0.8221	1.00	1.00
O 1-	6	0.2354	0.2252	0.6704	1.00	1.00
O 1-	7	0.8300	0.2809	0.6023	1.00	1.00
O 1-	8	0.9879	0.2088	0.4905	1.00	1.00
O 1-	9	0.0286	0.2818	0.6624	1.00	1.00
O 1-	10	0.8380	0.2500	0.0000	1.00	1.00
O 1-	11	0.0000	0.2604	0.1151	1.00	1.00
O 1-	12	0.1621	0.2500	0.0000	1.00	1.00
O 1-	13	0.5152	0.2460	0.8221	1.00	1.00
O 1-	14	0.6743	0.2242	0.3202	1.00	1.00
O 1-	15	0.6591	0.2381	0.5000	1.00	1.00
O 1-	16	0.8778	0.2918	0.3444	1.00	1.00
O 1-	17	0.1966	0.2353	0.1779	1.00	1.00
O 1-	18	0.0827	0.2252	0.3296	1.00	1.00
O 1-	19	0.4881	0.2809	0.3977	1.00	1.00
O 1-	20	0.3302	0.2088	0.5095	1.00	1.00
O 1-	21	0.2895	0.2818	0.3376	1.00	1.00
O 1-	22	0.8885	0.0000	0.0969	1.00	1.00
O 1-	23	0.0000	0.7397	0.1151	1.00	1.00
O 1-	24	0.1322	0.5000	0.1029	1.00	1.00
O 1-	25	0.5692	0.5000	0.7303	1.00	1.00
O 1-	26	0.5152	0.7540	0.8221	1.00	1.00
O 1-	27	0.6743	0.7758	0.3202	1.00	1.00
O 1-	28	0.5747	0.0000	0.4105	1.00	1.00
O 1-	29	0.9439	0.0000	0.3629	1.00	1.00
O 1-	30	0.8778	0.7082	0.3444	1.00	1.00
O 1-	31	0.1966	0.7647	0.1779	1.00	1.00
O 1-	32	0.0827	0.7748	0.3296	1.00	1.00
O 1-	33	0.2205	0.0000	0.2931	1.00	1.00
O 1-	34	0.4881	0.7192	0.3977	1.00	1.00
O 1-	35	0.3542	0.5000	0.4527	1.00	1.00
O 1-	36	0.3302	0.7912	0.5095	1.00	1.00
O 1-	37	0.2895	0.7182	0.3376	1.00	1.00
O 1-	38	0.4296	0.0000	0.9031	1.00	1.00
O 1-	39	0.3181	0.7397	0.8849	1.00	1.00

O 1-	40	0.1859	0.5000	0.8971	1.00	1.00
O 1-	41	0.7489	0.5000	0.2697	1.00	1.00
O 1-	42	0.8029	0.7540	0.1779	1.00	1.00
O 1-	43	0.6438	0.7758	0.6798	1.00	1.00
O 1-	44	0.6591	0.7619	0.5000	1.00	1.00
O 1-	45	0.8380	0.7500	0.0000	1.00	1.00
O 1-	46	0.7434	0.0000	0.5895	1.00	1.00
O 1-	47	0.3743	0.0000	0.6371	1.00	1.00
O 1-	48	0.4403	0.7082	0.6556	1.00	1.00
O 1-	49	0.1215	0.7647	0.8221	1.00	1.00
O 1-	50	0.2354	0.7748	0.6704	1.00	1.00
O 1-	51	0.0976	0.0000	0.7069	1.00	1.00
O 1-	52	0.8300	0.7192	0.6023	1.00	1.00
O 1-	53	0.9639	0.5000	0.5473	1.00	1.00
O 1-	54	0.9879	0.7912	0.4905	1.00	1.00
O 1-	55	0.0286	0.7182	0.6624	1.00	1.00
O 1-	56	0.1621	0.7500	0.0000	1.00	1.00

LAYER 3 {This is layer beta}
{consecutive stakings of this layer forms a monoclinic polymorph}
NONE

Si4+	1	0.5710	0.1866	0.9026	1.00	1.00
Si4+	2	0.8066	0.3129	0.8984	1.00	1.00
Si4+	3	0.2200	0.1851	0.2714	1.00	1.00
Si4+	4	0.2842	0.1898	0.5936	1.00	1.00
Si4+	5	0.8827	0.1806	0.7146	1.00	1.00
Si4+	6	0.0005	0.1802	0.3798	1.00	1.00
Si4+	7	0.5710	0.8134	0.9026	1.00	1.00
Si4+	8	0.0436	0.3168	0.5739	1.00	1.00
Si4+	9	0.8066	0.6871	0.8984	1.00	1.00
Si4+	10	0.1104	0.6866	0.0974	1.00	1.00
Si4+	11	0.8748	0.8129	0.1016	1.00	1.00
Si4+	12	0.4614	0.6851	0.7286	1.00	1.00
Si4+	13	0.3972	0.6898	0.4064	1.00	1.00
Si4+	14	0.7987	0.6806	0.2854	1.00	1.00
Si4+	15	0.6809	0.6802	0.6202	1.00	1.00
Si4+	16	0.6378	0.8168	0.4261	1.00	1.00
Si4+	17	0.2200	0.8149	0.2714	1.00	1.00
Si4+	18	0.2842	0.8102	0.5936	1.00	1.00
Si4+	19	0.1104	0.3134	0.0974	1.00	1.00
Si4+	20	0.8748	0.1871	0.1016	1.00	1.00
Si4+	21	0.8827	0.8194	0.7146	1.00	1.00
Si4+	22	0.4614	0.3149	0.7286	1.00	1.00
Si4+	23	0.3972	0.3102	0.4064	1.00	1.00
Si4+	24	0.7987	0.3194	0.2854	1.00	1.00
Si4+	25	0.6809	0.3198	0.6202	1.00	1.00
Si4+	26	0.6378	0.1832	0.4261	1.00	1.00
Si4+	27	0.0005	0.8198	0.3798	1.00	1.00
Si4+	28	0.0436	0.6832	0.5739	1.00	1.00
O 1-	1	0.0465	0.5000	0.5445	1.00	1.00
O 1-	2	0.6814	0.2772	0.8781	1.00	1.00
O 1-	3	0.1980	0.2803	0.1771	1.00	1.00
O 1-	4	0.3525	0.2504	0.6813	1.00	1.00
O 1-	5	0.8800	0.2242	0.8228	1.00	1.00
O 1-	6	0.1203	0.2107	0.3410	1.00	1.00
O 1-	7	0.1635	0.7410	0.5994	1.00	1.00
O 1-	8	0.9172	0.2970	0.3288	1.00	1.00
O 1-	9	-0.0020	0.2131	0.4893	1.00	1.00
O 1-	10	0.9663	0.2951	0.6622	1.00	1.00

O 1-	11	0.1635	0.2590	0.5994	1.00	1.00
O 1-	12	0.1558	0.7500	0.0000	1.00	1.00
O 1-	13	0.0000	0.7772	0.1219	1.00	1.00
O 1-	14	0.8441	0.7500	0.0000	1.00	1.00
O 1-	15	0.4834	0.7803	0.8229	1.00	1.00
O 1-	16	0.3289	0.7504	0.3187	1.00	1.00
O 1-	17	0.8015	0.7242	0.1772	1.00	1.00
O 1-	18	0.5611	0.7107	0.6590	1.00	1.00
O 1-	19	0.7642	0.7970	0.6712	1.00	1.00
O 1-	20	0.6834	0.7131	0.5107	1.00	1.00
O 1-	21	0.7152	0.7951	0.3378	1.00	1.00
O 1-	22	0.5179	0.7590	0.4006	1.00	1.00
O 1-	23	0.1558	0.2500	0.0000	1.00	1.00
O 1-	24	0.0878	0.5000	0.0904	1.00	1.00
O 1-	25	0.0000	0.2228	0.1219	1.00	1.00
O 1-	26	0.8441	0.2500	0.0000	1.00	1.00
O 1-	27	0.8535	0.0000	0.1072	1.00	1.00
O 1-	28	0.4486	0.5000	0.7510	1.00	1.00
O 1-	29	0.4834	0.2197	0.8229	1.00	1.00
O 1-	30	0.4015	0.5000	0.4060	1.00	1.00
O 1-	31	0.3407	0.2500	0.5000	1.00	1.00
O 1-	32	0.3289	0.2496	0.3187	1.00	1.00
O 1-	33	0.7611	0.5000	0.2979	1.00	1.00
O 1-	34	0.8015	0.2759	0.1772	1.00	1.00
O 1-	35	0.5611	0.2893	0.6590	1.00	1.00
O 1-	36	0.7151	0.5000	0.6399	1.00	1.00
O 1-	37	0.7642	0.2030	0.6712	1.00	1.00
O 1-	38	0.6834	0.2869	0.5107	1.00	1.00
O 1-	39	0.7152	0.2049	0.3378	1.00	1.00
O 1-	40	0.6349	0.0000	0.4555	1.00	1.00
O 1-	41	0.5179	0.2410	0.4006	1.00	1.00
O 1-	42	0.5937	0.0000	0.9096	1.00	1.00
O 1-	43	0.6814	0.7228	0.8781	1.00	1.00
O 1-	44	0.8279	0.5000	0.8928	1.00	1.00
O 1-	45	0.2328	0.0000	0.2490	1.00	1.00
O 1-	46	0.1980	0.7197	0.1771	1.00	1.00
O 1-	47	0.2799	0.0000	0.5940	1.00	1.00
O 1-	48	0.3407	0.7500	0.5000	1.00	1.00
O 1-	49	0.3525	0.7496	0.6813	1.00	1.00
O 1-	50	0.9203	0.0000	0.7021	1.00	1.00
O 1-	51	0.8800	0.7759	0.8228	1.00	1.00
O 1-	52	0.1203	0.7893	0.3410	1.00	1.00
O 1-	53	-0.0336	1.0000	0.3601	1.00	1.00
O 1-	54	0.9172	0.7030	0.3288	1.00	1.00
O 1-	55	-0.0020	0.7869	0.4893	1.00	1.00
O 1-	56	0.9663	0.7049	0.6622	1.00	1.00

LAYER 4 {layer beta'}

NONE						
Si4+	1	0.4358	0.8110	0.9025	1.00	1.00
Si4+	2	0.1954	0.6886	0.9011	1.00	1.00
Si4+	3	0.4358	0.1890	0.9025	1.00	1.00
Si4+	4	0.1954	0.3114	0.9011	1.00	1.00
Si4+	5	0.7760	0.3155	0.2781	1.00	1.00
Si4+	6	0.7191	0.1858	0.5929	1.00	1.00
Si4+	7	0.3450	0.1815	0.6181	1.00	1.00
Si4+	8	0.1208	0.1856	0.7155	1.00	1.00
Si4+	9	0.7760	0.6845	0.2781	1.00	1.00

Si4+	10	0.9526	0.3178	0.5756	1.00	1.00
Si4+	11	0.7191	0.8143	0.5929	1.00	1.00
Si4+	12	0.8823	0.1890	0.0975	1.00	1.00
Si4+	13	0.1227	0.3114	0.0989	1.00	1.00
Si4+	14	0.5421	0.3155	0.7219	1.00	1.00
Si4+	15	0.5990	0.1858	0.4071	1.00	1.00
Si4+	16	0.9731	0.1815	0.3819	1.00	1.00
Si4+	17	0.1973	0.1856	0.2845	1.00	1.00
Si4+	18	0.3655	0.3178	0.4244	1.00	1.00
Si4+	19	0.3450	0.8185	0.6181	1.00	1.00
Si4+	20	0.1208	0.8144	0.7155	1.00	1.00
Si4+	21	0.8823	0.8110	0.0975	1.00	1.00
Si4+	22	0.1227	0.6886	0.0989	1.00	1.00
Si4+	23	0.5421	0.6845	0.7219	1.00	1.00
Si4+	24	0.5990	0.8143	0.4071	1.00	1.00
Si4+	25	0.9526	0.6822	0.5756	1.00	1.00
Si4+	26	0.9731	0.8185	0.3819	1.00	1.00
Si4+	27	0.1973	0.8144	0.2845	1.00	1.00
Si4+	28	0.3655	0.6822	0.4244	1.00	1.00
O 1-	1	0.3181	0.2604	0.8849	1.00	1.00
O 1-	2	0.8029	0.2460	0.1779	1.00	1.00
O 1-	3	0.6438	0.2242	0.6798	1.00	1.00
O 1-	4	0.4403	0.2918	0.6556	1.00	1.00
O 1-	5	0.1215	0.2353	0.8221	1.00	1.00
O 1-	6	0.2354	0.2252	0.6704	1.00	1.00
O 1-	7	0.8300	0.2809	0.6023	1.00	1.00
O 1-	8	0.9879	0.2088	0.4905	1.00	1.00
O 1-	9	0.0286	0.2818	0.6624	1.00	1.00
O 1-	10	0.8380	0.2500	0.0000	1.00	1.00
O 1-	11	0.0000	0.2604	0.1151	1.00	1.00
O 1-	12	0.1621	0.2500	0.0000	1.00	1.00
O 1-	13	0.5152	0.2460	0.8221	1.00	1.00
O 1-	14	0.6743	0.2242	0.3202	1.00	1.00
O 1-	15	0.6591	0.2381	0.5000	1.00	1.00
O 1-	16	0.8778	0.2918	0.3444	1.00	1.00
O 1-	17	0.1966	0.2353	0.1779	1.00	1.00
O 1-	18	0.0827	0.2252	0.3296	1.00	1.00
O 1-	19	0.4881	0.2809	0.3977	1.00	1.00
O 1-	20	0.3302	0.2088	0.5095	1.00	1.00
O 1-	21	0.2895	0.2818	0.3376	1.00	1.00
O 1-	22	0.8885	0.0000	0.0969	1.00	1.00
O 1-	23	0.0000	0.7397	0.1151	1.00	1.00
O 1-	24	0.1322	0.5000	0.1029	1.00	1.00
O 1-	25	0.5692	0.5000	0.7303	1.00	1.00
O 1-	26	0.5152	0.7540	0.8221	1.00	1.00
O 1-	27	0.6743	0.7758	0.3202	1.00	1.00
O 1-	28	0.5747	0.0000	0.4105	1.00	1.00
O 1-	29	0.9439	0.0000	0.3629	1.00	1.00
O 1-	30	0.8778	0.7082	0.3444	1.00	1.00
O 1-	31	0.1966	0.7647	0.1779	1.00	1.00
O 1-	32	0.0827	0.7748	0.3296	1.00	1.00
O 1-	33	0.2205	0.0000	0.2931	1.00	1.00
O 1-	34	0.4881	0.7192	0.3977	1.00	1.00
O 1-	35	0.3542	0.5000	0.4527	1.00	1.00
O 1-	36	0.3302	0.7912	0.5095	1.00	1.00
O 1-	37	0.2895	0.7182	0.3376	1.00	1.00
O 1-	38	0.4296	0.0000	0.9031	1.00	1.00
O 1-	39	0.3181	0.7397	0.8849	1.00	1.00
O 1-	40	0.1859	0.5000	0.8971	1.00	1.00
O 1-	41	0.7489	0.5000	0.2697	1.00	1.00

O 1-	42	0.8029	0.7540	0.1779	1.00	1.00
O 1-	43	0.6438	0.7758	0.6798	1.00	1.00
O 1-	44	0.6591	0.7619	0.5000	1.00	1.00
O 1-	45	0.8380	0.7500	0.0000	1.00	1.00
O 1-	46	0.7434	0.0000	0.5895	1.00	1.00
O 1-	47	0.3743	0.0000	0.6371	1.00	1.00
O 1-	48	0.4403	0.7082	0.6556	1.00	1.00
O 1-	49	0.1215	0.7647	0.8221	1.00	1.00
O 1-	50	0.2354	0.7748	0.6704	1.00	1.00
O 1-	51	0.0976	0.0000	0.7069	1.00	1.00
O 1-	52	0.8300	0.7192	0.6023	1.00	1.00
O 1-	53	0.9639	0.5000	0.5473	1.00	1.00
O 1-	54	0.9879	0.7912	0.4905	1.00	1.00
O 1-	55	0.0286	0.7182	0.6624	1.00	1.00
O 1-	56	0.1621	0.7500	0.0000	1.00	1.00

STACKING
recursive
Infinite

TRANSITIONS

{layer 1}				
{to layer 1}	0.675	-0.3333	0.0	1.0
{to layer 2}	0.225	-0.3333	0.0	1.0
{to layer 3}	0.075	-0.3333	0.0	1.0
{to layer 4}	0.025	-0.3333	0.0	1.0
{layer 2}				
{to layer 1}	0.225	0.3333	0.0	1.0
{to layer 2}	0.675	0.3333	0.0	1.0
{to layer 3}	0.025	0.3333	0.0	1.0
{to layer 4}	0.075	0.3333	0.0	1.0
{layer 3}				
{to layer 1}	0.675	-0.3333	0.5	1.0
{to layer 2}	0.225	-0.3333	0.5	1.0
{to layer 3}	0.075	-0.3333	0.5	1.0
{to layer 4}	0.025	-0.3333	0.5	1.0
{layer 4}				
{to layer 1}	0.225	0.3333	0.5	1.0
{to layer 2}	0.675	0.3333	0.5	1.0
{to layer 3}	0.025	0.3333	0.5	1.0
{to layer 4}	0.075	0.3333	0.5	1.0

```
{THIS IS AN INPUT FILE FOR THE PROGRAM DIFFaX}
{This input file can be used to simulate intergrowths of layers gamma, gamma'}
{delta and delta'. This file has been provided as supplementary material for}
{the paper "A Model for the Structure of the Large-Pore Zeolite SSZ-31"}
{J. Am. Chem. Soc., 1997}
{See the text of the paper for more details}

{Layer 1= layer gamma}
{Layer 2= layer gamma'}
{Layer 3= layer delta}
{Layer 4= layer delta'}

{To simulate intergrowths of polymorphs E and F, }
{then the stacking transitions are defined as:}
{1-1  is a polymorph E stacking transition}
{1-2  is a polymorph F stacking transition}
{1-3 cannot occur}
{1-4 cannot occur}
{2-1  is a polymorph F stacking transition}
{2-2  is a polymorph E stacking transition}
{2-3 cannot occur}
{2-4 cannot occur}
{3-i cannot occur, i=1,2,3,4}
{4-i cannot occur, i=1,2,3,4}
{Remember that the program requires that the sum of the stacking}
{transitions for each layer equal to one}

{To simulate intergrowths of polymorphs G and H, }
{then the stacking transitions are defined as:}
{1-i cannot occur, i=1,2,3,4}
{2-i cannot occur, i=1,2,3,4}
{3-1 cannot occur}
{3-2 cannot occur}
{3-3  is a polymorph G stacking transition}
{3-4  is a polymorph H stacking transition}
{4-1 cannot occur}
{4-2 cannot occur}
{4-3  is a polymorph H stacking transition}
{4-4  is a polymorph G stacking transition}


INSTRUMENTAL
X-RAY
1.5418
NONE

STRUCTURAL
8.38  24.74  28.78  90.0 {}
UNKNOWN 1.0
4



LAYER 1  {layer gamma}
NONE
Si4+    1   0.3230  0.6428  0.3015  1.00    1.00
Si4+    2   0.1906  0.3946  0.4496  1.00    1.00
Si4+    3   0.1905  0.2734  0.4497  1.00    1.00
Si4+    4   0.3183  0.8401  0.3084  1.00    1.00
```

Si4+	5	0.3155	0.2375	0.3577	1.00	1.00
Si4+	6	0.1770	0.1428	0.3015	1.00	1.00
Si4+	7	0.3094	0.8946	0.4496	1.00	1.00
Si4+	8	0.8095	0.2734	0.4497	1.00	1.00
Si4+	9	0.8171	0.3937	0.1420	1.00	1.00
Si4+	10	0.6829	0.8937	0.1420	1.00	1.00
Si4+	11	0.8145	0.8107	0.2110	1.00	1.00
Si4+	12	0.6818	0.8401	0.3084	1.00	1.00
Si4+	13	0.6855	0.3107	0.2110	1.00	1.00
Si4+	14	0.6905	0.7734	0.4497	1.00	1.00
Si4+	15	0.8183	0.3401	0.3084	1.00	1.00
Si4+	16	0.8155	0.7375	0.3577	1.00	1.00
Si4+	17	0.6770	0.6428	0.3015	1.00	1.00
Si4+	18	0.8094	0.3946	0.4496	1.00	1.00
Si4+	19	0.6845	0.2375	0.3577	1.00	1.00
Si4+	20	0.6829	0.4406	0.3580	1.00	1.00
Si4+	21	0.8145	0.5235	0.2890	1.00	1.00
Si4+	22	0.1829	0.3937	0.1420	1.00	1.00
Si4+	23	0.3145	0.3107	0.2110	1.00	1.00
Si4+	24	0.1905	0.0609	0.0504	1.00	1.00
Si4+	25	0.3183	0.4942	0.1916	1.00	1.00
Si4+	26	0.3155	0.0968	0.1423	1.00	1.00
Si4+	27	0.1770	0.1915	0.1985	1.00	1.00
Si4+	28	0.3094	0.4397	0.0504	1.00	1.00
Si4+	29	0.8095	0.0609	0.0504	1.00	1.00
Si4+	30	0.6818	0.4942	0.1916	1.00	1.00
Si4+	31	0.1829	0.9406	0.3580	1.00	1.00
Si4+	32	0.6845	0.0968	0.1423	1.00	1.00
Si4+	33	0.3145	0.0235	0.2890	1.00	1.00
Si4+	34	0.8230	0.1915	0.1985	1.00	1.00
Si4+	35	0.6905	0.5609	0.0504	1.00	1.00
Si4+	36	0.6906	0.4397	0.0504	1.00	1.00
Si4+	37	0.8183	0.9942	0.1916	1.00	1.00
Si4+	38	0.8155	0.5968	0.1423	1.00	1.00
Si4+	39	0.6770	0.6915	0.1985	1.00	1.00
Si4+	40	0.8094	0.9397	0.0504	1.00	1.00
Si4+	41	0.3095	0.5609	0.0504	1.00	1.00
Si4+	42	0.1818	0.9942	0.1916	1.00	1.00
Si4+	43	0.1845	0.5968	0.1423	1.00	1.00
Si4+	44	0.3230	0.6915	0.1985	1.00	1.00
Si4+	45	0.1906	0.9397	0.0504	1.00	1.00
Si4+	46	0.3171	0.4406	0.3580	1.00	1.00
Si4+	47	0.1855	0.5235	0.2890	1.00	1.00
Si4+	48	0.3095	0.7734	0.4497	1.00	1.00
Si4+	49	0.8171	0.9406	0.3580	1.00	1.00
Si4+	50	0.6855	0.0235	0.2890	1.00	1.00
Si4+	51	0.8230	0.1428	0.3015	1.00	1.00
Si4+	52	0.1818	0.3401	0.3084	1.00	1.00
Si4+	53	0.3171	0.8937	0.1420	1.00	1.00
Si4+	54	0.1855	0.8107	0.2110	1.00	1.00
Si4+	55	0.6906	0.8946	0.4496	1.00	1.00
Si4+	56	0.1845	0.7375	0.3577	1.00	1.00
O 1-	1	0.5000	0.7707	0.4475	1.00	1.00
O 1-	2	0.7032	0.9502	0.1684	1.00	1.00
O 1-	3	0.7500	0.5794	0.0000	1.00	1.00
O 1-	4	0.7483	0.5003	0.0601	1.00	1.00
O 1-	5	0.7643	0.6003	0.0888	1.00	1.00
O 1-	6	0.7500	0.9211	0.0000	1.00	1.00
O 1-	7	0.7878	0.6542	0.1665	1.00	1.00
O 1-	8	0.7359	0.9003	0.0889	1.00	1.00

O 1-	9	0.7102	0.5518	0.1678	1.00	1.00
O 1-	10	0.7191	0.8359	0.2540	1.00	1.00
O 1-	11	0.7918	0.8488	0.1665	1.00	1.00
O 1-	12	0.7473	0.7516	0.1999	1.00	1.00
O 1-	13	0.7032	0.3841	0.3316	1.00	1.00
O 1-	14	0.7483	0.8340	0.4399	1.00	1.00
O 1-	15	0.7643	0.7339	0.4112	1.00	1.00
O 1-	16	0.7878	0.6800	0.3335	1.00	1.00
O 1-	17	0.6725	0.6671	0.2500	1.00	1.00
O 1-	18	0.7359	0.4340	0.4111	1.00	1.00
O 1-	19	0.7102	0.7825	0.3322	1.00	1.00
O 1-	20	0.7191	0.4984	0.2460	1.00	1.00
O 1-	21	0.7918	0.4855	0.3335	1.00	1.00
O 1-	22	0.7473	0.5827	0.3001	1.00	1.00
O 1-	23	0.2500	0.0794	0.0000	1.00	1.00
O 1-	24	0.2500	0.4211	0.0000	1.00	1.00
O 1-	25	0.7500	0.0794	0.0000	1.00	1.00
O 1-	26	0.5000	0.4370	0.0525	1.00	1.00
O 1-	27	0.7500	0.4211	0.0000	1.00	1.00
O 1-	28	0.5000	0.8973	0.4475	1.00	1.00
O 1-	29	0.0000	0.0635	0.0525	1.00	1.00
O 1-	30	0.5000	0.4591	0.3558	1.00	1.00
O 1-	31	0.0000	0.3580	0.3157	1.00	1.00
O 1-	32	0.2968	0.3841	0.3316	1.00	1.00
O 1-	33	0.2517	0.8340	0.4399	1.00	1.00
O 1-	34	0.0000	0.5274	0.2764	1.00	1.00
O 1-	35	0.0000	0.7535	0.3543	1.00	1.00
O 1-	36	0.2357	0.7339	0.4112	1.00	1.00
O 1-	37	0.2122	0.6800	0.3335	1.00	1.00
O 1-	38	0.2641	0.4340	0.4111	1.00	1.00
O 1-	39	0.5000	0.6416	0.3223	1.00	1.00
O 1-	40	0.2898	0.7825	0.3322	1.00	1.00
O 1-	41	0.2809	0.4984	0.2460	1.00	1.00
O 1-	42	0.2082	0.4855	0.3335	1.00	1.00
O 1-	43	0.0000	0.2707	0.4475	1.00	1.00
O 1-	44	0.2527	0.5827	0.3001	1.00	1.00
O 1-	45	0.5000	0.8752	0.1442	1.00	1.00
O 1-	46	0.0000	0.9762	0.1843	1.00	1.00
O 1-	47	0.2968	0.9502	0.1684	1.00	1.00
O 1-	48	0.2500	0.5794	0.0000	1.00	1.00
O 1-	49	0.2517	0.5003	0.0601	1.00	1.00
O 1-	50	0.0000	0.8069	0.2236	1.00	1.00
O 1-	51	0.0000	0.5807	0.1457	1.00	1.00
O 1-	52	0.2357	0.6003	0.0888	1.00	1.00
O 1-	53	0.2500	0.9211	0.0000	1.00	1.00
O 1-	54	0.2122	0.6542	0.1665	1.00	1.00
O 1-	55	0.3275	0.6671	0.2500	1.00	1.00
O 1-	56	0.2032	0.4502	0.1684	1.00	1.00
O 1-	57	0.2483	0.0003	0.0601	1.00	1.00
O 1-	58	0.2641	0.9003	0.0889	1.00	1.00
O 1-	59	0.2643	0.1003	0.0888	1.00	1.00
O 1-	60	0.2878	0.1542	0.1665	1.00	1.00
O 1-	61	0.2359	0.4003	0.0889	1.00	1.00
O 1-	62	0.2102	0.0518	0.1678	1.00	1.00
O 1-	63	0.2191	0.3359	0.2540	1.00	1.00
O 1-	64	0.2918	0.3488	0.1665	1.00	1.00
O 1-	65	0.2473	0.2516	0.1999	1.00	1.00
O 1-	66	0.2032	0.8841	0.3316	1.00	1.00
O 1-	67	0.5000	0.6927	0.1777	1.00	1.00
O 1-	68	0.2483	0.3340	0.4399	1.00	1.00

O 1-	69	0.2643	0.2339	0.4112	1.00	1.00
O 1-	70	0.2878	0.1800	0.3335	1.00	1.00
O 1-	71	0.1725	0.1671	0.2500	1.00	1.00
O 1-	72	0.2359	0.9340	0.4111	1.00	1.00
O 1-	73	0.2102	0.2825	0.3322	1.00	1.00
O 1-	74	0.2191	-0.0017	0.2460	1.00	1.00
O 1-	75	0.2918	0.9855	0.3335	1.00	1.00
O 1-	76	0.2473	0.0827	0.3001	1.00	1.00
O 1-	77	0.0000	0.9370	0.0525	1.00	1.00
O 1-	78	0.5000	0.5635	0.0525	1.00	1.00
O 1-	79	0.0000	0.9591	0.3558	1.00	1.00
O 1-	80	0.5000	0.8580	0.3157	1.00	1.00
O 1-	81	0.7968	0.8841	0.3316	1.00	1.00
O 1-	82	0.7517	0.3340	0.4399	1.00	1.00
O 1-	83	0.5000	0.0274	0.2764	1.00	1.00
O 1-	84	0.5000	0.2535	0.3543	1.00	1.00
O 1-	85	0.7357	0.2339	0.4112	1.00	1.00
O 1-	86	0.2898	0.5518	0.1678	1.00	1.00
O 1-	87	0.7122	0.1800	0.3335	1.00	1.00
O 1-	88	0.7641	0.9340	0.4111	1.00	1.00
O 1-	89	0.0000	0.1416	0.3223	1.00	1.00
O 1-	90	0.7898	0.2825	0.3322	1.00	1.00
O 1-	91	0.7809	-0.0017	0.2460	1.00	1.00
O 1-	92	0.7082	0.9855	0.3335	1.00	1.00
O 1-	93	0.7527	0.0827	0.3001	1.00	1.00
O 1-	94	0.0000	0.3752	0.1442	1.00	1.00
O 1-	95	0.2809	0.8359	0.2540	1.00	1.00
O 1-	96	0.5000	0.4762	0.1843	1.00	1.00
O 1-	97	0.7968	0.4502	0.1684	1.00	1.00
O 1-	98	0.7517	0.0003	0.0601	1.00	1.00
O 1-	99	0.5000	0.3069	0.2236	1.00	1.00
O 1-	100	0.5000	0.0807	0.1457	1.00	1.00
O 1-	101	0.7357	0.1003	0.0888	1.00	1.00
O 1-	102	0.7122	0.1542	0.1665	1.00	1.00
O 1-	103	0.8275	0.1671	0.2500	1.00	1.00
O 1-	104	0.7641	0.4003	0.0889	1.00	1.00
O 1-	105	0.0000	0.1927	0.1777	1.00	1.00
O 1-	106	0.2082	0.8488	0.1665	1.00	1.00
O 1-	107	0.7898	0.0518	0.1678	1.00	1.00
O 1-	108	0.7809	0.3359	0.2540	1.00	1.00
O 1-	109	0.7082	0.3488	0.1665	1.00	1.00
O 1-	110	0.7527	0.2516	0.1999	1.00	1.00
O 1-	111	0.0000	0.3973	0.4475	1.00	1.00
O 1-	112	0.2527	0.7516	0.1999	1.00	1.00

LAYER 2 {layer gamma'}
NONE

Si4+	1	0.8155	0.2628	0.3577	1.00	1.00
Si4+	2	0.8183	0.6602	0.3084	1.00	1.00
Si4+	3	0.6905	0.2269	0.4497	1.00	1.00
Si4+	4	0.8094	0.0606	0.0504	1.00	1.00
Si4+	5	0.6770	0.3088	0.1985	1.00	1.00
Si4+	6	0.8155	0.4035	0.1423	1.00	1.00
Si4+	7	0.8183	0.0061	0.1916	1.00	1.00
Si4+	8	0.6905	0.4394	0.0504	1.00	1.00
Si4+	9	0.3094	0.1057	0.4496	1.00	1.00
Si4+	10	0.1770	0.8575	0.3015	1.00	1.00
Si4+	11	0.3155	0.7628	0.3577	1.00	1.00

Si4+	12	0.3145	0.9767	0.2890	1.00	1.00
Si4+	13	0.3183	0.1602	0.3084	1.00	1.00
Si4+	14	0.1829	0.0597	0.3580	1.00	1.00
Si4+	15	0.1905	0.7269	0.4497	1.00	1.00
Si4+	16	0.3094	0.5606	0.0504	1.00	1.00
Si4+	17	0.1770	0.8088	0.1985	1.00	1.00
Si4+	18	0.3155	0.9035	0.1423	1.00	1.00
Si4+	19	0.3183	0.5061	0.1916	1.00	1.00
Si4+	20	0.1905	0.9394	0.0504	1.00	1.00
Si4+	21	0.8145	0.4767	0.2890	1.00	1.00
Si4+	22	0.6855	0.9767	0.2890	1.00	1.00
Si4+	23	0.6829	0.5597	0.3580	1.00	1.00
Si4+	24	0.8171	0.0597	0.3580	1.00	1.00
Si4+	25	0.1906	0.0606	0.0504	1.00	1.00
Si4+	26	0.3230	0.3088	0.1985	1.00	1.00
Si4+	27	0.8145	0.1895	0.2110	1.00	1.00
Si4+	28	0.1845	0.4035	0.1423	1.00	1.00
Si4+	29	0.1818	0.0061	0.1916	1.00	1.00
Si4+	30	0.3095	0.4394	0.0504	1.00	1.00
Si4+	31	0.1906	0.6057	0.4496	1.00	1.00
Si4+	32	0.3230	0.3575	0.3015	1.00	1.00
Si4+	33	0.1845	0.2628	0.3577	1.00	1.00
Si4+	34	0.1855	0.4767	0.2890	1.00	1.00
Si4+	35	0.1818	0.6602	0.3084	1.00	1.00
Si4+	36	0.3171	0.5597	0.3580	1.00	1.00
Si4+	37	0.3095	0.2269	0.4497	1.00	1.00
Si4+	38	0.6829	0.1066	0.1420	1.00	1.00
Si4+	39	0.8094	0.6057	0.4496	1.00	1.00
Si4+	40	0.6855	0.6895	0.2110	1.00	1.00
Si4+	41	0.8171	0.6066	0.1420	1.00	1.00
Si4+	42	0.6906	0.5606	0.0504	1.00	1.00
Si4+	43	0.8230	0.8088	0.1985	1.00	1.00
Si4+	44	0.6845	0.9035	0.1423	1.00	1.00
Si4+	45	0.6818	0.5061	0.1916	1.00	1.00
Si4+	46	0.6770	0.3575	0.3015	1.00	1.00
Si4+	47	0.8095	0.9394	0.0504	1.00	1.00
Si4+	48	0.6906	0.1057	0.4496	1.00	1.00
Si4+	49	0.8230	0.8575	0.3015	1.00	1.00
Si4+	50	0.6845	0.7628	0.3577	1.00	1.00
Si4+	51	0.6818	0.1602	0.3084	1.00	1.00
Si4+	52	0.8095	0.7269	0.4497	1.00	1.00
Si4+	53	0.1855	0.1895	0.2110	1.00	1.00
Si4+	54	0.3171	0.1066	0.1420	1.00	1.00
Si4+	55	0.3145	0.6895	0.2110	1.00	1.00
Si4+	56	0.1829	0.6066	0.1420	1.00	1.00
O 1-	1	0.7473	0.2487	0.1999	1.00	1.00
O 1-	2	0.7878	0.3460	0.1665	1.00	1.00
O 1-	3	0.5000	0.9195	0.1457	1.00	1.00
O 1-	4	0.5000	0.6934	0.2236	1.00	1.00
O 1-	5	0.2483	0.0000	0.0601	1.00	1.00
O 1-	6	0.2032	0.5501	0.1684	1.00	1.00
O 1-	7	0.5000	0.5240	0.1843	1.00	1.00
O 1-	8	0.0000	0.6251	0.1442	1.00	1.00
O 1-	9	0.5000	0.2295	0.4475	1.00	1.00
O 1-	10	0.0000	0.6030	0.4475	1.00	1.00
O 1-	11	0.7500	0.0792	0.0000	1.00	1.00
O 1-	12	0.5000	0.4367	0.0525	1.00	1.00
O 1-	13	0.0000	0.0633	0.0525	1.00	1.00
O 1-	14	0.7643	0.3999	0.0888	1.00	1.00
O 1-	15	0.2473	0.9176	0.3001	1.00	1.00

O 1-	16	0.2918	0.0148	0.3335	1.00	1.00
O 1-	17	0.2191	0.0019	0.2460	1.00	1.00
O 1-	18	0.2102	0.7178	0.3322	1.00	1.00
O 1-	19	0.0000	0.8587	0.3223	1.00	1.00
O 1-	20	0.2359	0.0663	0.4111	1.00	1.00
O 1-	21	0.2878	0.8202	0.3335	1.00	1.00
O 1-	22	0.2643	0.7663	0.4112	1.00	1.00
O 1-	23	0.0000	0.4195	0.1457	1.00	1.00
O 1-	24	0.5000	0.7467	0.3543	1.00	1.00
O 1-	25	0.5000	0.9729	0.2764	1.00	1.00
O 1-	26	0.2483	0.6663	0.4399	1.00	1.00
O 1-	27	0.2032	0.1162	0.3316	1.00	1.00
O 1-	28	0.5000	0.1422	0.3157	1.00	1.00
O 1-	29	0.0000	0.0412	0.3558	1.00	1.00
O 1-	30	0.7527	0.9176	0.3001	1.00	1.00
O 1-	31	0.7082	0.0148	0.3335	1.00	1.00
O 1-	32	0.7809	0.0019	0.2460	1.00	1.00
O 1-	33	0.7898	0.7178	0.3322	1.00	1.00
O 1-	34	0.0000	0.1934	0.2236	1.00	1.00
O 1-	35	0.7641	0.0663	0.4111	1.00	1.00
O 1-	36	0.8275	0.8331	0.2500	1.00	1.00
O 1-	37	0.7122	0.8202	0.3335	1.00	1.00
O 1-	38	0.7357	0.7663	0.4112	1.00	1.00
O 1-	39	0.7517	0.6663	0.4399	1.00	1.00
O 1-	40	0.7968	0.1162	0.3316	1.00	1.00
O 1-	41	0.7483	0.5000	0.0601	1.00	1.00
O 1-	42	0.7527	0.7487	0.1999	1.00	1.00
O 1-	43	0.7082	0.6515	0.1665	1.00	1.00
O 1-	44	0.7500	0.4208	0.0000	1.00	1.00
O 1-	45	0.7809	0.6644	0.2540	1.00	1.00
O 1-	46	0.7898	0.9485	0.1678	1.00	1.00
O 1-	47	0.7641	0.6000	0.0889	1.00	1.00
O 1-	48	0.7122	0.8460	0.1665	1.00	1.00
O 1-	49	0.7357	0.8999	0.0888	1.00	1.00
O 1-	50	0.7517	0.0000	0.0601	1.00	1.00
O 1-	51	0.7968	0.5501	0.1684	1.00	1.00
O 1-	52	0.7032	0.0501	0.1684	1.00	1.00
O 1-	53	0.0000	0.0240	0.1843	1.00	1.00
O 1-	54	0.5000	0.1251	0.1442	1.00	1.00
O 1-	55	0.7918	0.1515	0.1665	1.00	1.00
O 1-	56	0.0000	0.7295	0.4475	1.00	1.00
O 1-	57	0.5000	0.1030	0.4475	1.00	1.00
O 1-	58	0.0000	0.9367	0.0525	1.00	1.00
O 1-	59	0.7191	0.1644	0.2540	1.00	1.00
O 1-	60	0.2500	0.5792	0.0000	1.00	1.00
O 1-	61	0.5000	0.5633	0.0525	1.00	1.00
O 1-	62	0.2500	0.9208	0.0000	1.00	1.00
O 1-	63	0.7473	0.4176	0.3001	1.00	1.00
O 1-	64	0.7918	0.5148	0.3335	1.00	1.00
O 1-	65	0.7191	0.5019	0.2460	1.00	1.00
O 1-	66	0.7102	0.2178	0.3322	1.00	1.00
O 1-	67	0.7102	0.4485	0.1678	1.00	1.00
O 1-	68	0.5000	0.3587	0.3223	1.00	1.00
O 1-	69	0.7359	0.5663	0.4111	1.00	1.00
O 1-	70	0.7878	0.3202	0.3335	1.00	1.00
O 1-	71	0.7643	0.2663	0.4112	1.00	1.00
O 1-	72	0.0000	0.2467	0.3543	1.00	1.00
O 1-	73	0.0000	0.4729	0.2764	1.00	1.00
O 1-	74	0.7483	0.1663	0.4399	1.00	1.00
O 1-	75	0.7032	0.6162	0.3316	1.00	1.00

O 1-	76	0.0000	0.6422	0.3157	1.00	1.00
O 1-	77	0.5000	0.5412	0.3558	1.00	1.00
O 1-	78	0.2527	0.4176	0.3001	1.00	1.00
O 1-	79	0.2082	0.5148	0.3335	1.00	1.00
O 1-	80	0.2809	0.5019	0.2460	1.00	1.00
O 1-	81	0.2898	0.2178	0.3322	1.00	1.00
O 1-	82	0.2641	0.5663	0.4111	1.00	1.00
O 1-	83	0.3275	0.3331	0.2500	1.00	1.00
O 1-	84	0.2122	0.3202	0.3335	1.00	1.00
O 1-	85	0.2357	0.2663	0.4112	1.00	1.00
O 1-	86	0.2517	0.1663	0.4399	1.00	1.00
O 1-	87	0.2968	0.6162	0.3316	1.00	1.00
O 1-	88	0.7500	0.5792	0.0000	1.00	1.00
O 1-	89	0.7500	0.9208	0.0000	1.00	1.00
O 1-	90	0.5000	0.3076	0.1777	1.00	1.00
O 1-	91	0.2527	0.2487	0.1999	1.00	1.00
O 1-	92	0.2082	0.1515	0.1665	1.00	1.00
O 1-	93	0.2809	0.1644	0.2540	1.00	1.00
O 1-	94	0.2898	0.4485	0.1678	1.00	1.00
O 1-	95	0.7359	0.1000	0.0889	1.00	1.00
O 1-	96	0.2641	0.1000	0.0889	1.00	1.00
O 1-	97	0.2122	0.3460	0.1665	1.00	1.00
O 1-	98	0.2500	0.0792	0.0000	1.00	1.00
O 1-	99	0.2357	0.3999	0.0888	1.00	1.00
O 1-	100	0.2517	0.5000	0.0601	1.00	1.00
O 1-	101	0.2500	0.4208	0.0000	1.00	1.00
O 1-	102	0.2968	0.0501	0.1684	1.00	1.00
O 1-	103	0.2473	0.7487	0.1999	1.00	1.00
O 1-	104	0.6725	0.3331	0.2500	1.00	1.00
O 1-	105	0.2918	0.6515	0.1665	1.00	1.00
O 1-	106	0.2191	0.6644	0.2540	1.00	1.00
O 1-	107	0.2102	0.9485	0.1678	1.00	1.00
O 1-	108	0.0000	0.8076	0.1777	1.00	1.00
O 1-	109	0.2359	0.6000	0.0889	1.00	1.00
O 1-	110	0.1725	0.8331	0.2500	1.00	1.00
O 1-	111	0.2878	0.8460	0.1665	1.00	1.00
O 1-	112	0.2643	0.8999	0.0888	1.00	1.00

LAYER 3 {layer delta}

NONE

Si4+	1	0.3195	0.2741	0.4503	1.00	1.00
Si4+	2	0.1853	0.8386	0.3006	1.00	1.00
Si4+	3	0.1828	0.2415	0.3558	1.00	1.00
Si4+	4	0.3118	0.1474	0.2999	1.00	1.00
Si4+	5	0.1805	0.9027	0.4503	1.00	1.00
Si4+	6	0.1805	0.7741	0.4503	1.00	1.00
Si4+	7	0.3147	0.3386	0.3006	1.00	1.00
Si4+	8	0.3172	0.7415	0.3558	1.00	1.00
Si4+	9	0.1882	0.6474	0.2999	1.00	1.00
Si4+	10	0.3195	0.4027	0.4503	1.00	1.00
Si4+	11	0.6833	0.8937	0.1439	1.00	1.00
Si4+	12	0.8145	0.8049	0.2046	1.00	1.00
Si4+	13	0.8195	0.7741	0.4503	1.00	1.00
Si4+	14	0.6805	0.2741	0.4503	1.00	1.00
Si4+	15	0.8147	0.8386	0.3006	1.00	1.00
Si4+	16	0.8172	0.2415	0.3558	1.00	1.00
Si4+	17	0.6833	0.9399	0.3561	1.00	1.00
Si4+	18	0.6882	0.1474	0.2999	1.00	1.00
Si4+	19	0.8145	0.0287	0.2954	1.00	1.00

Si4+	20	0.8195	0.9027	0.4503	1.00	1.00
Si4+	21	0.6853	0.3386	0.3006	1.00	1.00
Si4+	22	0.1805	0.0595	0.0497	1.00	1.00
Si4+	23	0.3147	0.4950	0.1994	1.00	1.00
Si4+	24	0.1833	0.3937	0.1439	1.00	1.00
Si4+	25	0.3172	0.0921	0.1443	1.00	1.00
Si4+	26	0.3145	0.3049	0.2046	1.00	1.00
Si4+	27	0.1882	0.1862	0.2002	1.00	1.00
Si4+	28	0.3195	0.4309	0.0497	1.00	1.00
Si4+	29	0.8195	0.0595	0.0497	1.00	1.00
Si4+	30	0.6853	0.4950	0.1994	1.00	1.00
Si4+	31	0.6828	0.0921	0.1443	1.00	1.00
Si4+	32	0.6828	0.7415	0.3558	1.00	1.00
Si4+	33	0.1833	0.4399	0.3561	1.00	1.00
Si4+	34	0.3145	0.5287	0.2954	1.00	1.00
Si4+	35	0.8118	0.1862	0.2002	1.00	1.00
Si4+	36	0.6805	0.4309	0.0497	1.00	1.00
Si4+	37	0.6805	0.5595	0.0497	1.00	1.00
Si4+	38	0.8147	0.9950	0.1994	1.00	1.00
Si4+	39	0.8172	0.5921	0.1443	1.00	1.00
Si4+	40	0.6882	0.6862	0.2002	1.00	1.00
Si4+	41	0.8195	0.9309	0.0497	1.00	1.00
Si4+	42	0.3195	0.5595	0.0497	1.00	1.00
Si4+	43	0.1853	0.9950	0.1994	1.00	1.00
Si4+	44	0.1828	0.5921	0.1443	1.00	1.00
Si4+	45	0.3167	0.9399	0.3561	1.00	1.00
Si4+	46	0.1855	0.0287	0.2954	1.00	1.00
Si4+	47	0.3118	0.6862	0.2002	1.00	1.00
Si4+	48	0.1805	0.9309	0.0497	1.00	1.00
Si4+	49	0.8167	0.3937	0.1439	1.00	1.00
Si4+	50	0.8118	0.6474	0.2999	1.00	1.00
Si4+	51	0.6855	0.3049	0.2046	1.00	1.00
Si4+	52	0.8167	0.4399	0.3561	1.00	1.00
Si4+	53	0.6855	0.5287	0.2954	1.00	1.00
Si4+	54	0.3167	0.8937	0.1439	1.00	1.00
Si4+	55	0.1855	0.8049	0.2046	1.00	1.00
Si4+	56	0.6805	0.4027	0.4503	1.00	1.00
O 1-	1	0.7057	0.3452	0.1615	1.00	1.00
O 1-	2	0.7748	0.2492	0.1936	1.00	1.00
O 1-	3	0.0000	0.9232	0.4458	1.00	1.00
O 1-	4	0.5000	0.2536	0.4458	1.00	1.00
O 1-	5	0.2057	0.8452	0.1615	1.00	1.00
O 1-	6	0.7250	0.9476	0.1722	1.00	1.00
O 1-	7	0.7500	0.5763	0.0000	1.00	1.00
O 1-	8	0.6858	0.4952	0.0551	1.00	1.00
O 1-	9	0.7867	0.5867	0.0896	1.00	1.00
O 1-	10	0.7500	0.9141	0.0000	1.00	1.00
O 1-	11	0.7776	0.6525	0.1605	1.00	1.00
O 1-	12	0.2748	0.7492	0.1936	1.00	1.00
O 1-	13	0.7500	0.6668	0.2500	1.00	1.00
O 1-	14	0.7136	0.9037	0.0897	1.00	1.00
O 1-	15	0.7044	0.5505	0.1713	1.00	1.00
O 1-	16	0.7383	0.8319	0.2500	1.00	1.00
O 1-	17	0.7943	0.8452	0.1615	1.00	1.00
O 1-	18	0.7253	0.7492	0.1936	1.00	1.00
O 1-	19	0.7250	0.8861	0.3278	1.00	1.00
O 1-	20	0.6858	0.3384	0.4449	1.00	1.00
O 1-	21	0.7867	0.2469	0.4104	1.00	1.00
O 1-	22	0.7776	0.1811	0.3395	1.00	1.00
O 1-	23	0.7500	0.1668	0.2500	1.00	1.00

O	1-	24	0.7136	0.9299	0.4103	1.00	1.00
O	1-	25	0.7044	0.2831	0.3287	1.00	1.00
O	1-	26	0.7383	0.0017	0.2500	1.00	1.00
O	1-	27	0.7943	0.9884	0.3385	1.00	1.00
O	1-	28	0.7253	0.0844	0.3064	1.00	1.00
O	1-	29	0.2500	0.0763	0.0000	1.00	1.00
O	1-	30	0.2500	0.4141	0.0000	1.00	1.00
O	1-	31	0.7500	0.0763	0.0000	1.00	1.00
O	1-	32	0.5000	0.4104	0.0542	1.00	1.00
O	1-	33	0.7500	0.4141	0.0000	1.00	1.00
O	1-	34	0.0000	0.0800	0.0542	1.00	1.00
O	1-	35	0.5000	0.9553	0.3479	1.00	1.00
O	1-	36	0.0000	0.8531	0.2958	1.00	1.00
O	1-	37	0.2750	0.8861	0.3278	1.00	1.00
O	1-	38	0.3142	0.3384	0.4449	1.00	1.00
O	1-	39	0.5000	0.4232	0.4458	1.00	1.00
O	1-	40	0.0000	0.0401	0.2867	1.00	1.00
O	1-	41	0.0000	0.2549	0.3446	1.00	1.00
O	1-	42	0.2133	0.2469	0.4104	1.00	1.00
O	1-	43	0.2224	0.1811	0.3395	1.00	1.00
O	1-	44	0.2500	0.1668	0.2500	1.00	1.00
O	1-	45	0.2864	0.9299	0.4103	1.00	1.00
O	1-	46	0.5000	0.1574	0.3036	1.00	1.00
O	1-	47	0.2956	0.2831	0.3287	1.00	1.00
O	1-	48	0.0000	0.7536	0.4458	1.00	1.00
O	1-	49	0.2617	0.0017	0.2500	1.00	1.00
O	1-	50	0.2057	0.9884	0.3385	1.00	1.00
O	1-	51	0.2748	0.0844	0.3064	1.00	1.00
O	1-	52	0.5000	0.8783	0.1521	1.00	1.00
O	1-	53	0.0000	0.9805	0.2042	1.00	1.00
O	1-	54	0.2750	0.9476	0.1722	1.00	1.00
O	1-	55	0.2500	0.5763	0.0000	1.00	1.00
O	1-	56	0.3142	0.4952	0.0551	1.00	1.00
O	1-	57	0.0000	0.7936	0.2133	1.00	1.00
O	1-	58	0.0000	0.5787	0.1554	1.00	1.00
O	1-	59	0.2133	0.5867	0.0896	1.00	1.00
O	1-	60	0.2500	0.9141	0.0000	1.00	1.00
O	1-	61	0.2224	0.6525	0.1605	1.00	1.00
O	1-	62	0.2250	0.4476	0.1722	1.00	1.00
O	1-	63	0.1858	0.9952	0.0551	1.00	1.00
O	1-	64	0.2867	0.0867	0.0896	1.00	1.00
O	1-	65	0.2776	0.1525	0.1605	1.00	1.00
O	1-	66	0.2500	0.6668	0.2500	1.00	1.00
O	1-	67	0.2136	0.4037	0.0897	1.00	1.00
O	1-	68	0.2044	0.0505	0.1713	1.00	1.00
O	1-	69	0.2383	0.3319	0.2500	1.00	1.00
O	1-	70	0.2943	0.3452	0.1615	1.00	1.00
O	1-	71	0.2253	0.2492	0.1936	1.00	1.00
O	1-	72	0.2250	0.3861	0.3278	1.00	1.00
O	1-	73	0.1858	0.8384	0.4449	1.00	1.00
O	1-	74	0.2867	0.7469	0.4104	1.00	1.00
O	1-	75	0.2864	0.9037	0.0897	1.00	1.00
O	1-	76	0.2776	0.6811	0.3395	1.00	1.00
O	1-	77	0.2136	0.4299	0.4103	1.00	1.00
O	1-	78	0.2044	0.7831	0.3287	1.00	1.00
O	1-	79	0.2383	0.5017	0.2500	1.00	1.00
O	1-	80	0.2943	0.4884	0.3385	1.00	1.00
O	1-	81	0.2253	0.5844	0.3064	1.00	1.00
O	1-	82	0.5000	0.6762	0.1964	1.00	1.00
O	1-	83	0.0000	0.9104	0.0542	1.00	1.00

O 1-	84	0.5000	0.5800	0.0542	1.00	1.00
O 1-	85	0.0000	0.4553	0.3479	1.00	1.00
O 1-	86	0.5000	0.3531	0.2958	1.00	1.00
O 1-	87	0.7750	0.3861	0.3278	1.00	1.00
O 1-	88	0.8142	0.8384	0.4449	1.00	1.00
O 1-	89	0.5000	0.5401	0.2867	1.00	1.00
O 1-	90	0.5000	0.7549	0.3446	1.00	1.00
O 1-	91	0.7133	0.7469	0.4104	1.00	1.00
O 1-	92	0.7224	0.6811	0.3395	1.00	1.00
O 1-	93	0.7864	0.4299	0.4103	1.00	1.00
O 1-	94	0.0000	0.6574	0.3036	1.00	1.00
O 1-	95	0.7956	0.7831	0.3287	1.00	1.00
O 1-	96	0.7617	0.5017	0.2500	1.00	1.00
O 1-	97	0.7057	0.4884	0.3385	1.00	1.00
O 1-	98	0.7748	0.5844	0.3064	1.00	1.00
O 1-	99	0.0000	0.3783	0.1521	1.00	1.00
O 1-	100	0.5000	0.4805	0.2042	1.00	1.00
O 1-	101	0.7750	0.4476	0.1722	1.00	1.00
O 1-	102	0.8142	0.9952	0.0551	1.00	1.00
O 1-	103	0.2956	0.5505	0.1713	1.00	1.00
O 1-	104	0.5000	0.2936	0.2133	1.00	1.00
O 1-	105	0.5000	0.0787	0.1554	1.00	1.00
O 1-	106	0.7133	0.0867	0.0896	1.00	1.00
O 1-	107	0.7224	0.1525	0.1605	1.00	1.00
O 1-	108	0.7864	0.4037	0.0897	1.00	1.00
O 1-	109	0.0000	0.1762	0.1964	1.00	1.00
O 1-	110	0.7956	0.0505	0.1713	1.00	1.00
O 1-	111	0.7617	0.3319	0.2500	1.00	1.00
O 1-	112	0.2617	0.8319	0.2500	1.00	1.00

LAYER 4 {layer delta'}

NONE

Si4+	1	0.1833	0.6066	0.1439	1.00	1.00
Si4+	2	0.3145	0.6954	0.2046	1.00	1.00
Si4+	3	0.3167	0.1066	0.1439	1.00	1.00
Si4+	4	0.1855	0.1954	0.2046	1.00	1.00
Si4+	5	0.6882	0.8529	0.2999	1.00	1.00
Si4+	6	0.8195	0.2262	0.4503	1.00	1.00
Si4+	7	0.6853	0.6617	0.3006	1.00	1.00
Si4+	8	0.6828	0.2588	0.3558	1.00	1.00
Si4+	9	0.8118	0.3529	0.2999	1.00	1.00
Si4+	10	0.6805	0.5976	0.4503	1.00	1.00
Si4+	11	0.8195	0.9408	0.0497	1.00	1.00
Si4+	12	0.6853	0.5053	0.1994	1.00	1.00
Si4+	13	0.8195	0.0976	0.4503	1.00	1.00
Si4+	14	0.6828	0.9082	0.1443	1.00	1.00
Si4+	15	0.8118	0.8141	0.2002	1.00	1.00
Si4+	16	0.6805	0.5694	0.0497	1.00	1.00
Si4+	17	0.8167	0.6066	0.1439	1.00	1.00
Si4+	18	0.6855	0.6954	0.2046	1.00	1.00
Si4+	19	0.6833	0.1066	0.1439	1.00	1.00
Si4+	20	0.3167	0.0604	0.3561	1.00	1.00
Si4+	21	0.1855	0.9716	0.2954	1.00	1.00
Si4+	22	0.3195	0.7262	0.4503	1.00	1.00
Si4+	23	0.1853	0.1617	0.3006	1.00	1.00
Si4+	24	0.1828	0.7588	0.3558	1.00	1.00
Si4+	25	0.3118	0.8529	0.2999	1.00	1.00
Si4+	26	0.1805	0.0976	0.4503	1.00	1.00
Si4+	27	0.3195	0.4408	0.0497	1.00	1.00

Si4+	28	0.1853	0.0053	0.1994	1.00	1.00
Si4+	29	0.1828	0.4082	0.1443	1.00	1.00
Si4+	30	0.8145	0.1954	0.2046	1.00	1.00
Si4+	31	0.3118	0.3141	0.2002	1.00	1.00
Si4+	32	0.1805	0.0694	0.0497	1.00	1.00
Si4+	33	0.8167	0.5604	0.3561	1.00	1.00
Si4+	34	0.6833	0.0604	0.3561	1.00	1.00
Si4+	35	0.6855	0.4716	0.2954	1.00	1.00
Si4+	36	0.8145	0.9716	0.2954	1.00	1.00
Si4+	37	0.1805	0.9408	0.0497	1.00	1.00
Si4+	38	0.3147	0.5053	0.1994	1.00	1.00
Si4+	39	0.3172	0.9082	0.1443	1.00	1.00
Si4+	40	0.1882	0.8141	0.2002	1.00	1.00
Si4+	41	0.3195	0.5694	0.0497	1.00	1.00
Si4+	42	0.1805	0.2262	0.4503	1.00	1.00
Si4+	43	0.1833	0.5604	0.3561	1.00	1.00
Si4+	44	0.3147	0.6617	0.3006	1.00	1.00
Si4+	45	0.3145	0.4716	0.2954	1.00	1.00
Si4+	46	0.3172	0.2588	0.3558	1.00	1.00
Si4+	47	0.1882	0.3529	0.2999	1.00	1.00
Si4+	48	0.3195	0.5976	0.4503	1.00	1.00
Si4+	49	0.6805	0.4408	0.0497	1.00	1.00
Si4+	50	0.8147	0.0053	0.1994	1.00	1.00
Si4+	51	0.8172	0.4082	0.1443	1.00	1.00
Si4+	52	0.6882	0.3141	0.2002	1.00	1.00
Si4+	53	0.8195	0.0694	0.0497	1.00	1.00
Si4+	54	0.6805	0.7262	0.4503	1.00	1.00
Si4+	55	0.8147	0.1617	0.3006	1.00	1.00
Si4+	56	0.8172	0.7588	0.3558	1.00	1.00
O 1-	1	0.2776	0.8478	0.1605	1.00	1.00
O 1-	2	0.2136	0.5966	0.0897	1.00	1.00
O 1-	3	0.0000	0.8241	0.1964	1.00	1.00
O 1-	4	0.2044	0.9498	0.1713	1.00	1.00
O 1-	5	0.2383	0.6684	0.2500	1.00	1.00
O 1-	6	0.2943	0.6551	0.1615	1.00	1.00
O 1-	7	0.2253	0.7511	0.1936	1.00	1.00
O 1-	8	0.2750	0.0528	0.1722	1.00	1.00
O 1-	9	0.7500	0.3335	0.2500	1.00	1.00
O 1-	10	0.2500	0.4241	0.0000	1.00	1.00
O 1-	11	0.3142	0.5051	0.0551	1.00	1.00
O 1-	12	0.2133	0.4136	0.0896	1.00	1.00
O 1-	13	0.2500	0.0862	0.0000	1.00	1.00
O 1-	14	0.2224	0.3478	0.1605	1.00	1.00
O 1-	15	0.2500	0.3335	0.2500	1.00	1.00
O 1-	16	0.2864	0.0966	0.0897	1.00	1.00
O 1-	17	0.2956	0.4498	0.1713	1.00	1.00
O 1-	18	0.7136	0.0966	0.0897	1.00	1.00
O 1-	19	0.2617	0.1684	0.2500	1.00	1.00
O 1-	20	0.2057	0.1551	0.1615	1.00	1.00
O 1-	21	0.2748	0.2511	0.1936	1.00	1.00
O 1-	22	0.5000	0.3241	0.1964	1.00	1.00
O 1-	23	0.7500	0.9241	0.0000	1.00	1.00
O 1-	24	0.7500	0.5862	0.0000	1.00	1.00
O 1-	25	0.2750	0.1143	0.3278	1.00	1.00
O 1-	26	0.3142	0.6619	0.4449	1.00	1.00
O 1-	27	0.2133	0.7534	0.4104	1.00	1.00
O 1-	28	0.2224	0.8192	0.3395	1.00	1.00
O 1-	29	0.2500	0.8335	0.2500	1.00	1.00
O 1-	30	0.2864	0.0704	0.4103	1.00	1.00
O 1-	31	0.2956	0.7172	0.3287	1.00	1.00

O	1-	32	0.2617	-0.0014	0.2500	1.00	1.00
O	1-	33	0.2057	0.0119	0.3385	1.00	1.00
O	1-	34	0.2748	0.9159	0.3064	1.00	1.00
O	1-	35	0.5000	0.0450	0.3479	1.00	1.00
O	1-	36	0.0000	0.1472	0.2958	1.00	1.00
O	1-	37	0.7250	0.1143	0.3278	1.00	1.00
O	1-	38	0.6858	0.6619	0.4449	1.00	1.00
O	1-	39	0.0000	0.9603	0.2867	1.00	1.00
O	1-	40	0.0000	0.7454	0.3446	1.00	1.00
O	1-	41	0.7867	0.7534	0.4104	1.00	1.00
O	1-	42	0.7776	0.8192	0.3395	1.00	1.00
O	1-	43	0.7500	0.8335	0.2500	1.00	1.00
O	1-	44	0.7136	0.0704	0.4103	1.00	1.00
O	1-	45	0.5000	0.8429	0.3036	1.00	1.00
O	1-	46	0.7044	0.4498	0.1713	1.00	1.00
O	1-	47	0.7044	0.7172	0.3287	1.00	1.00
O	1-	48	0.7383	-0.0014	0.2500	1.00	1.00
O	1-	49	0.7943	0.0119	0.3385	1.00	1.00
O	1-	50	0.7253	0.9159	0.3064	1.00	1.00
O	1-	51	0.2500	0.9241	0.0000	1.00	1.00
O	1-	52	0.5000	0.5899	0.0542	1.00	1.00
O	1-	53	0.2500	0.5862	0.0000	1.00	1.00
O	1-	54	0.7383	0.1684	0.2500	1.00	1.00
O	1-	55	0.0000	0.9203	0.0542	1.00	1.00
O	1-	56	0.5000	0.5771	0.4458	1.00	1.00
O	1-	57	0.0000	0.2467	0.4458	1.00	1.00
O	1-	58	0.7943	0.1551	0.1615	1.00	1.00
O	1-	59	0.5000	0.1220	0.1521	1.00	1.00
O	1-	60	0.0000	0.0198	0.2042	1.00	1.00
O	1-	61	0.7250	0.0528	0.1722	1.00	1.00
O	1-	62	0.7750	0.5528	0.1722	1.00	1.00
O	1-	63	0.8142	0.0051	0.0551	1.00	1.00
O	1-	64	0.7133	0.9136	0.0896	1.00	1.00
O	1-	65	0.7224	0.8478	0.1605	1.00	1.00
O	1-	66	0.7864	0.5966	0.0897	1.00	1.00
O	1-	67	0.7956	0.9498	0.1713	1.00	1.00
O	1-	68	0.7617	0.6684	0.2500	1.00	1.00
O	1-	69	0.7500	0.4241	0.0000	1.00	1.00
O	1-	70	0.7057	0.6551	0.1615	1.00	1.00
O	1-	71	0.7748	0.7511	0.1936	1.00	1.00
O	1-	72	0.6858	0.5051	0.0551	1.00	1.00
O	1-	73	0.7750	0.6143	0.3278	1.00	1.00
O	1-	74	0.8142	0.1619	0.4449	1.00	1.00
O	1-	75	0.7133	0.2534	0.4104	1.00	1.00
O	1-	76	0.7224	0.3192	0.3395	1.00	1.00
O	1-	77	0.7864	0.5704	0.4103	1.00	1.00
O	1-	78	0.7956	0.2172	0.3287	1.00	1.00
O	1-	79	0.0000	0.2068	0.2133	1.00	1.00
O	1-	80	0.7617	0.4986	0.2500	1.00	1.00
O	1-	81	0.7057	0.5119	0.3385	1.00	1.00
O	1-	82	0.7748	0.4159	0.3064	1.00	1.00
O	1-	83	0.0000	0.5450	0.3479	1.00	1.00
O	1-	84	0.5000	0.6472	0.2958	1.00	1.00
O	1-	85	0.2250	0.6143	0.3278	1.00	1.00
O	1-	86	0.1858	0.1619	0.4449	1.00	1.00
O	1-	87	0.5000	0.4603	0.2867	1.00	1.00
O	1-	88	0.5000	0.2454	0.3446	1.00	1.00
O	1-	89	0.2867	0.2534	0.4104	1.00	1.00
O	1-	90	0.0000	0.4216	0.1554	1.00	1.00
O	1-	91	0.2776	0.3192	0.3395	1.00	1.00

```
O 1-     92  0.2136  0.5704  0.4103  1.00    1.00
O 1-     93  0.0000  0.3429  0.3036  1.00    1.00
O 1-     94  0.2044  0.2172  0.3287  1.00    1.00
O 1-     95  0.2383  0.4986  0.2500  1.00    1.00
O 1-     96  0.2943  0.5119  0.3385  1.00    1.00
O 1-     97  0.2253  0.4159  0.3064  1.00    1.00
O 1-     98  0.7867  0.4136  0.0896  1.00    1.00
O 1-     99  0.0000  0.0899  0.0542  1.00    1.00
O 1-     100 0.5000  0.4203  0.0542  1.00    1.00
O 1-     101 0.0000  0.0771  0.4458  1.00    1.00
O 1-     102 0.7500  0.0862  0.0000  1.00    1.00
O 1-     103 0.5000  0.7467  0.4458  1.00    1.00
O 1-     104 0.0000  0.6220  0.1521  1.00    1.00
O 1-     105 0.5000  0.5198  0.2042  1.00    1.00
O 1-     106 0.2250  0.5528  0.1722  1.00    1.00
O 1-     107 0.1858  0.0051  0.0551  1.00    1.00
O 1-     108 0.5000  0.7068  0.2133  1.00    1.00
O 1-     109 0.5000  0.9216  0.1554  1.00    1.00
O 1-     110 0.2867  0.9136  0.0896  1.00    1.00
O 1-     111 0.7776  0.3478  0.1605  1.00    1.00
O 1-     112 0.7253  0.2511  0.1936  1.00    1.00
```

```
STACKING
recursive
infinite

TRANSITIONS

{layer 1}
{to layer 1} 0.000    0.0  -0.1667    0.5
{to layer 2} 0.000    0.0  -0.1667    0.5
{to layer 3} 0.999    0.0  -0.1667    0.5
{to layer 4} 0.001    0.0  -0.1667    0.5

{layer 2}
{to layer 1} 0.000    0.0   0.1667    0.5
{to layer 2} 0.000    0.0   0.1667    0.5
{to layer 3} 0.999    0.0   0.1667    0.5
{to layer 4} 0.001    0.0   0.1667    0.5

{layer 3}
{to layer 1} 0.000    0.5  -0.1667    0.5
{to layer 2} 0.000    0.5  -0.1667    0.5
{to layer 3} 0.900    0.5  -0.1667    0.5
{to layer 4} 0.100    0.5  -0.1667    0.5

{layer 4}
{to layer 1} 0.000    0.5   0.1667    0.5
{to layer 2} 0.000    0.5   0.1667    0.5
{to layer 3} 0.100    0.5   0.1667    0.5
{to layer 4} 0.900    0.5   0.1667    0.5
```